METHODS OF IDENTIFYING MODULATORS OF BROMODOMAINS

FIELD OF THE INVENTION

The present invention provides the three-dimensional structure of a histone acetyltransferase bromodomain. The three-dimensional structural information is included in the invention. The present invention also identifies for the first time, that bromodomains can bind to an acetylated binding partners. The interaction between bromodomains and their binding partners play a crucial role in various cellular functions, including in the regulation/modulation of DNA transcription. Therefore, the present invention provides procedures for identifying agents that can modulate the interaction of bromodomains and their binding partners by high throughput drug screening and/or through the use of rational drug design based on the three-dimensional data provided herein.

BACKGROUND OF THE INVENTION

In recent years great strides have been made in the elucidation of the steps involved in intercellular and intracellular signaling. Indeed, the individual steps of the cascade of events involved in a number of cellular signal transduction processes have been determined. For example, intercellular signal transduction generally begins with an intercellular ligand binding the extracellular portion of a receptor of the plasma membrane. The bound receptor then either directly or indirectly initiates the activation of one or more cellular factors. An activated cellular factor may act as transcription factor by entering the nucleus to interact with its corresponding genomic response element, or alternatively, it may interact with other cellular factors depending on the complexity of the process. In either case, one or more transcription factors ultimately bind to one or more specific genomic response elements. This binding plays a crucial role in the up and/or down regulation of the transcription of the specific genes that are under the control of these genomic response elements. However, the process of re-organizing the chromatin of eukaryotic cells, which is a prerequisite for the binding of the transcription factor to the genomic response elements, has remained a mystery.

Chromatin contains several highly conserved histone proteins including: H3, H4, H2A, H2B, and H1. These histone proteins package eukaryotic DNA into repeating nucleosomal units that are folded into higher-order chromatin fibers [Luger and Richmond, *Curr. Opin. Genet. Dev.* **8:**140-146 (1998)]. A portion of the histone that comprises roughly a quarter of the protein protrudes from the chromatin surface, and is thereby sensitive to proteolytic enzymes [van Holde, in *Chromatin* (Rich, A,. *ed.*, Springer, New York) pages111-148 (1988); Hect *et al.*, *Cell* **80**:583-592 (1995)]. This portion of the histone is known as the "histone tail". Histone tails tend to be free for protein-protein interaction, and are also the portion of the histone most prone to post-translational modification. Such post-translational modification includes acetylation, phosphorylation, methylation, ubiquitination, and ADP-ribosylation [van Holde, in *Chromatin* (Rich, A,. *ed.*, Springer, New York) pages111-148 (1988)].

Of all classes of proteins, histones are amongst the most susceptible to post-translational modification. Perhaps the best studied post-translational modification of histones is the acetylation of specific lysine residues [Grunstin, M., *Nature*, **389:**349-352 (1997)]. Indeed, acetylation of histone lysine residues has been suggested to play a pivotal role in chromatin remodeling and gene activation. Consistently, distinct classes of enzymes, namely histone acetyltransferases (HATs) and histone deacetylases (HDACs), acetylate or de-acetylate specific histone lysine residues [Struhl, *Genes Dev.* **12**:599-606 (1998)].

Nearly all known nuclear HATs contain an approximately 110 amino acid sequence known as the bromodomain [Jeanmougin *et al.*, Trends in Biochemical *Sciences*, **22:**151-153 (1997)], a protein motif that was initially discovered in Drosophila brahma protein. Bromodomains are found in a large number of chromatin-associated proteins and have now been identified in approximately 40 proteins, often adjacent to other protein motifs [Jeanmougin *et al.*, *Trends in Biochemical Sciences*, **22:**151-153 (1997); Tamkun *et al.*, *Cell*, **68:**561-572 (1992): Hanes *et al.*, *Nucleic Acids Research*, **20:**2603 (1992)]. Proteins that contain a bromodomain often contain a second bromodomain. However, despite the wide occurrence of bromodomains and their

likely role in chromatin regulation, their three-dimensional structure and binding partners heretofore have remained unknown.

Therefore, there is a need to identify a binding partner for a bromodomain. In addition, there is a need to identify agonists or antagonists to the bromodomain-binding partner complex. Since a preferred method of drug-screening relies on structure based drug design, there is also a need to determine the three-dimensional structure of a bromodomain. In this case, once the three dimensional structure of bromodomain is determined, potential agonists and/or potential antagonists can be designed with the aid of computer modeling [Bugg *et al.*, *Scientific American*, **Dec.**:92-98 (1993); West *et al.*, *TIPS*, **16**:67-74 (1995); Dunbrack *et al.*, *Folding & Design*, **2**:27-42 (1997)]. However, heretofore the three-dimensional structure of the bromodomain has remained unknown. Therefore, there is a need for obtaining a form of the bromodomain that is amenable for NMR analysis and/or X-ray crystallographic analysis. Furthermore, there is a need for the determination of the three-dimensional structure of the bromodomain. Finally, there is a need for procedures for related structural based drug design predicated on such structural data.

The citation of any reference herein should not be construed as an admission that such reference is available as "Prior Art" to the instant application.

SUMMARY OF THE INVENTION

The present invention provides, for the first time, that bromodomains bind to acetyl-lysine residues of proteins. The present invention also provides the three-dimensional structure of a bromodomain as well as the three-dimensional structure of a bromodomain-acetyl-histamine complex. The structural information provided can be employed in methods of identifying drugs that can modulate the cellular processes that involve bromodomain-acetyl-lysine interactions. These interactions include chromatin remodeling, which is a required step in eukaryotic transcription. In a particular embodiment, the three-dimensional structural information is used in the design of an inhibitor of leukemia.

The present invention provides an isolated nucleic acid that encodes a peptide consisting of about 21 to 40 amino acids that comprises a ZA loop of a bromodomain. In a preferred embodiment the peptide comprises about 23 to 34 amino acids. The isolated nucleic acid can further comprise a heterologous nucleotide sequence.

In a preferred embodiment the peptide comprises the amino acid sequence of SEQ ID NO:3. In another embodiment the peptide comprises the amino acid sequence of SEQ ID NO:43. In particular embodiments the ZA loop is obtained from the bromodomain having the amino acid sequence of SEQ ID NO:7, or SEQ ID NO:8, or SEQ ID NO:9, or SEQ ID NO:10, or SEQ ID NO:11, or SEQ ID NO:12, or SEQ ID NO:13, or SEQ ID NO:14, or SEQ ID NO:15, or SEQ ID NO:16, or SEQ ID NO:17, or SEQ ID NO:18, or SEQ ID NO:19, or SEQ ID NO:20, or SEQ ID NO:21,or SEQ ID NO: 22, or SEQ ID NO:23, or SEQ ID NO:24, or SEQ ID NO:25, or SEQ ID NO:26, or SEQ ID NO:27, or SEQ ID NO:28, or SEQ ID NO:29, or SEQ ID NO:30, or SEQ ID NO: or SEQ ID NO:31, or SEQ ID NO:32,or SEQ ID NO: 33, or SEQ ID NO:34, or SEQ ID NO:35, or SEQ ID NO:36 , or SEQ ID NO:37, or SEQ ID NO:38, or SEQ ID NO: or SEQ ID NO:39, or SEQ ID NO:40, or SEQ ID NO:41, or SEQ ID NO:42.

The present invention further provides a recombinant DNA molecule that comprises an isolated nucleic acid of the present invention, as described above, with or without a heterologous nucleotide sequence. Such a recombinant DNA molecule can be operatively linked to an expression control sequence and can be part of an expression vector. The present invention further provides a cell that comprises such an expression vector. The cell can be either a eukaryotic or a prokaryotic cell. The present invention further provides a method of expressing the peptides of the present invention or fragments thereof in this cell. One such method comprises culturing the cell in an appropriate cell culture medium under conditions that provide for expression of the peptide by the cell.

The present invention further provides a peptide consisting of about 21 to 40 amino acids that comprises a ZA loop of a bromodomain. In a preferred embodiment the

peptide comprises about 23 to 34 amino acids. The present invention also provides fusion proteins or peptides comprising these peptides.

In a preferred embodiment the peptide comprises the amino acid sequence of SEQ ID NO:3. In another embodiment the peptide comprises the amino acid sequence of SEQ ID NO:43. In particular embodiments the ZA loop is obtained from the bromodomain having the amino acid sequence of SEQ ID NO:7, or SEQ ID NO:8, or SEQ ID NO:9, or SEQ ID NO:10, or SEQ ID NO:11, or SEQ ID NO:12, or SEQ ID NO:13, or SEQ ID NO:14, or SEQ ID NO:15, or SEQ ID NO:16, or SEQ ID NO:17, or SEQ ID NO:18, or SEQ ID NO:19, or SEQ ID NO:20, or SEQ ID NO:21,or SEQ ID NO: 22, or SEQ ID NO:23, or SEQ ID NO:24, or SEQ ID NO:25, or SEQ ID NO:26, or SEQ ID NO:27, or SEQ ID NO:28, or SEQ ID NO:29, or SEQ ID NO:30, or SEQ ID NO: or SEQ ID NO:31, or SEQ ID NO:32,or SEQ ID NO: 33, or SEQ ID NO:34, or SEQ ID NO:35, or SEQ ID NO:36 , or SEQ ID NO:37, or SEQ ID NO:38, or SEQ ID NO: or SEQ ID NO:39, or SEQ ID NO:40, or SEQ ID NO:41, or SEQ ID NO:42.

The present invention also provides antibodies raised against the peptides/proteins of the present invention, or raised against an antigenic fragment of these proteins/fragments. In a particular embodiment an antibody is raised against a fragment of the ZA loop of a bromodomain. In another embodiment an antibody is raised against a fragment of a protein or peptide that comprises an acetyl-lysine, wherein the protein or peptide can bind to a bromodomain. Such fragments can be conjugated to a carrier protein or be part of a fusion protein. In one embodiment the antibody is a polyclonal antibody. In another embodiment, the antibody is a monoclonal antibody. A hybridoma that makes the monoclonal antibody is also part of the present invention. In a particular embodiment the antibody is a chimeric antibody. Antibodies that can specifically recognize acetyl-lysine residues involved bromodomain binding are also part of the present invention.

In another aspect of the present invention a method is provided for identifying a compound that modulates the affinity of a bromodomain for a ligand (and/or protein) that comprises an acetylated lysine. One such embodiment comprises contacting the

bromodomain and the ligand in the presence of a compound under conditions that , the bromodomain and the ligand bind in the absence of the compound. The affinity of the bromodomain for the ligand is then determined (*e.g.*, measured). A compound is identified as a compound that modulates the affinty of the bromodomain for the ligand when there is a change in the affinity of the bromodomain for the ligand in the presence of the compound. When the affinity of the bromodomain for the ligand increases in the presence of the compound, the compound is identified as a promoting agent for the bromodomain-ligand complex. When the affinity of the bromodomain for the ligand decreases in the presence of the compound, the compound is identified as an inhibitor of the bromodomain-ligand complex. In a preferred embodiment, the compound to be tested is pre-selected by performing rational drug design with the set of atomic coordinates obtained from one or more of Tables 1-6. More preferably the selecting is performed in conjunction with computer modeling. In a particular embodiment, the compound is selected by performing rational drug design with the set of atomic coordinates obtained from a set of atomic coordinates defining the three-dimensional structure of a bromodomain consisting of the amino acid sequence of SEQ ID NO:7 alone or with acetyl-histamine.

The present invention also provides a method of identifying a compound that modulates the stability of a bromodomain-acetyl-lysine binding complex. One such embodiment comprises contacting the bromodomain-acetyl-lysine binding complex in the presence of the compound under conditions in which the bromodomain-acetyl-lysine binding complex forms in the absence of the compound. The stability of the bromodomain-acetyl-lysine binding complex is then determined (*e.g.*, measured). A compound is identified as a compound that modulates the stability of the bromodomain-acetyl-lysine binding complex, when there is a change in the stability of the bromodomain-acetyl-lysine binding complex in the presence of that compound. When the stability of the bromodomain-acetyl-lysine binding complex increases in the presence of the compound, the compound is identified as a stabilizing agent. When the stability of the bromodomain-acetyl-lysine binding complex decreases in the presence of the compound, the compound is identified as an inhibitor. In a preferred embodiment, the compound to be tested is pre-selected by performing rational drug

design with the set of atomic coordinates obtained from one or more of Tables 1-6. More preferably the selecting is performed in conjunction with computer modeling. In a particular embodiment, the compound is selected by performing rational drug design with the set of atomic coordinates obtained from a set of atomic coordinates defining the three-dimensional structure of a bromodomain consisting of the amino acid sequence of SEQ ID NO:7 alone or with acetyl-histamine.

As anyone having skill in the art of drug development would readily understand, the potential drugs selected by the above methodologies can be refined by re-testing in appropriate drug assays, including those disclosed herein. Chemical analogs of such potential drugs can be obtained (either through chemical synthesis or drug libraries) and be analogously tested. Therefore, methods comprising successive iterations of the steps of the individual drug assays, as exemplified herein, using either repetitive or different binding studies, or transcription activation studies or other such studies are envisioned in the present invention. In addition, potential drugs may be identified first by rapid throughput drug screening, as described below, prior to performing computer modeling on a potential drug using the three-dimensional structure of the bromodomain.

The present invention further comprises all of the potential, selected, and putative compounds (drugs) identified by the methods of the present invention, as well as the final drugs themselves identified with the methods of the present invention.

The present invention further provides a method for identifying a potential binding partner for a protein (*e.g.*, a histone) comprising an acetyl-lysine. One such embodiment comprises contacting the protein with a polypeptide comprising a bromodomain. In a preferred embodiment the bromodomain comprises the amino acid sequence of SEQ ID NO:3. In particular embodiments the bromodomain has the amino acid sequence of SEQ ID NO:7, or SEQ ID NO:8, or SEQ ID NO:9, or SEQ ID NO:10, or SEQ ID NO:11, or SEQ ID NO:12, or SEQ ID NO:13, or SEQ ID NO:14, or SEQ ID NO:15, or SEQ ID NO:16, or SEQ ID NO:17, or SEQ ID NO:18, or SEQ ID NO:19, or SEQ ID NO:20, or SEQ ID NO:21,or SEQ ID NO: 22, or SEQ ID

NO:23, or SEQ ID NO:24, or SEQ ID NO:25, or SEQ ID NO:26, or SEQ ID NO:27, or SEQ ID NO:28, or SEQ ID NO:29, or SEQ ID NO:30, or SEQ ID NO: or SEQ ID NO:31, or SEQ ID NO:32,or SEQ ID NO: 33, or SEQ ID NO:34, or SEQ ID NO:35, or SEQ ID NO:36 , or SEQ ID NO:37, or SEQ ID NO:38, or SEQ ID NO: or SEQ ID NO:39, or SEQ ID NO:40, or SEQ ID NO:41, or SEQ ID NO:42.

The present invention further provides a method for identifying a protein having a bromodomain. One such embodiment comprises contacting a cellular extract with a peptide comprising an acetyl-lysine.

The present invention further provides agents that can inhibit the binding of a bromodomain with a protein comprising an acetyl-lysine. In one embodiment the agent is ISYGR-*AcK*-KRRQRR (SEQ ID NO:4). In another embodiment the agent is ARKSTGG-A*cK*-APRKQL (SEQ ID NO:5). In still another embodiment the agent is QSTSRHK-*AcK*-LMFKTE (SEQ ID NO:6). In yet another embodiment the agent is an analog of acetyl-lysine such as acetyl-histamine. In still another embodiment the agent is an antibody that recognizes an acetyl-lysine of a protein binding partner of a bromodomain. In a preferred embodiment the agent is an antibody raised against a ZA loop of a bromodomain. These agents can be used as pharmaceuticals in compositions that contain a pharmaceutically acceptable carrier for example, or in the various drug assays of the present invention, serving as controls to demonstrate specificity.

Accordingly, it is a principal object of the present invention to provide the three-dimensional coordinates of a bromodomain.

It is a further object of the present invention to provide the three-dimensional coordinates of a bromodomain complexed with acetyl-histamine.

It is a further object of the present invention to provide an assay for identifying proteins that contain bromodomains that bind proteins that comprise acetyl-lysine.

It is a further object of the present invention to provide methods of identifying drugs that can modulate the bromodomain-acetyl-lysine binding complex.

It is a further object of the present invention to provide methods of identifying drugs that can inhibit the binding of a bromodomain to a protein containing acetyl-lysine.

It is a further object of the present invention to provide methods that incorporate the use of rational design for identifying such drugs.

It is a further object of the present invention to provide a method of identifying drugs that can treat leukemia.

It is a further object of the present invention to provide a method of identifying drugs that can treat and/or prevent AIDS.

These and other aspects of the present invention will be better appreciated by reference to the following drawings and Detailed Description.

BRIEF DESCRIPTION OF THE DRAWINGS

Figure 1. Structure-based sequence alignment of a selected number of bromodomains. The sequences were aligned based on the NMR-derived structure of the P/CAF bromodomain, and the predicated four α-helices are shown in green boxes. Bromodomains are grouped on the basis of the sequence and/or functional similarities as described by Jeanmougin *et al.*, [Trends in Biochemical *Sciences*, **22**:151-153 (1997)]. Residue numbers of the P/CAF bromodomain are indicated above its sequence. Three absolutely conserved residues, corresponding to Pro751, Pro767, and Asn803 in the P/CAF bromodomain, are shown in red. Highly conserved residues are colored in blue. The residues of the P/CAF bromodomain that interact with acetyl-histamine, as determined by intermolecular NOEs, are indicated by asterisks. The ZA loop, which is critical for acetyl-lysine binding, for each of the indicated bromodomains is also identified. The underlined residues were changed individually

by site-directed mutagenesis to Ala. Genbank accession numbers for the proteins are as indicated in Table 8, in the Example below, along with the SEQ ID NOs. for the bromodomain sequences.

Figures 2A-2H depict the structure of the P/CAF bromodomain. Figures 2A-2B shows the stereoview of the C_α trace of 30 superimposed NMR-derived structures of the bromodomain (residues 722-830). The N-terminal four residues (SKEP) which are structurally disordered are omitted for clarity. For the final 30 structures, the root-mean-square deviations (RMSDs) of the backbone and all heavy atoms are 0.63 ± 0.11Å and 1.15 ± 0.12Å for residues 723-830, respectively. The RMSDs of the backbone and all heavy atoms for the four α-helices (residues 727-743, 770-776, 785-802, and 807-827), are 0.34 ± 0.04Å and 0.87 ± 0.06Å, respectively. Figures 2C-2D show the stereoview of the bromodomain structures from the bottom of the protein, which is rotated approximately 90° from the orientation in Figures 2A-2B. Figure 2E shows the Ribbons [Carson, M., *J. Appl. Crystallogr.* **24**:958-961 (1991)] depiction of the averaged minimized NMR structure of the P/CAF bromodomain. The orientation of Figure 2E is as shown in Figures 2A-2B. Figures 2F-2G are schematic representations of the overall topology of the up-and-down four-helix bundle folds with the opposite handedness. The left-handed fold is seen in bromodomain, cytochrome b_5, and T4 lysozyme (left, Figure 2F), whereas the right-handed four-helix bundles are observed in proteins such as hemerythrin and cytochrome b_{562} (right, Figure 2G) [Richardson, J., *Adv.Protein Chem.*, **34**:167-339 (1989); Presnell and Cohen, *Proc. Natl. Acad. Sci. USA* **86**:6592-6596 (1989)]. Figure 2H is a molecular surface representation of the electrostatic potential (blue = positive; red = negative) of the bromodomain calculated in GRASP [Nicholls *et al.*, *Biophys. J.* **64**:166-170 (1993)]. The hydrophobic and aromatic residues (Tyr809, Tyr802, Tyr760, Ala757, and Val752) located between the ZA and BC loops are indicated.

Figures 3A-3C show the binding of the P/CAF bromodomain to AcK. Figure 3A shows the superimposed region of the 2D ^{15}N-HSQC spectra of the bromodomain (approximately 0.5 mM) in its free form (red) and complexed to the AcK-containing

H4 peptide (molar ratio 1:6) (black). Figure 3B is the Ribbon and dotted-surface diagram of the bromodomain depicting the location of the lysine-acetylated H4 peptide binding site. The color coding reflects the chemical shift changes ($\Delta\delta$) of the backbone amide ^{1}H and ^{15}N resonances upon binding to the AcK peptide as observed in the ^{15}N-HSQC spectra. The normalized weighted average of the chemical shift changes was calculated by $\Delta_{av}/\Delta_{max} = [\Delta\delta^{2}_{NH} + \Delta\delta^{2}_{N}/25)/2]^{1/2}/\Delta_{max}$, where Δ_{max} is the maximum weighted chemical shift difference observed for Tyr809 (0.16ppm). The backbone atoms are color-coded in red, yellow, or green for residues that have Δ_{av}/Δ_{max} of >0.6 (Tyr809, Glu808, Asn803, and Ala757), 0.2-0.6 (Ala813, Tyr802, Tyr760, and Val752), or <0.2 (Cys812, Ser807, Cys799, Phe796, and Phe748), respectively. The non-perturbed residues are shown in blue. Figure 3C shows the chemical structures of acetyl-lysine, acetyl-histamine, and acetyl-histidine.

Figure 4 depicts the acetyl-lysine binding pocket. This is the Ribbons [Carson, M., *J. Appl. Crystallogr.* **24**:958-961 (1991)] depiction of a portion of the P/CAF bromodomain complexed with the acetyl-histamine. The ligand is color-coded by atom type.

DETAILED DESCRIPTION OF THE INVENTION

The present invention identifies a general binding partner (ligand) for the protein motif known as the bromodomain. Indeed, by combining structural and site-directed mutagenesis studies the present invention demonstrates that bromodomains can interact specifically with acetyl-lysine (AcK), making them the first protein modules known to exhibit such interactions. Like other modular domains, such as Src homology-2 (SH2) and phosphotyrosine binding (PTB) domains, which specifically interact with phosphotyrosine-containing proteins, the bromodomain/acetyl-lysine recognition provides a means to regulate protein-protein interactions via protein lysine acetylation. The nature of the acetyl-lysine recognition by the bromodomain is similar to that of histone acetyltransferase interaction with acetyl-CoA. The present invention therefore couples for the first time, the functionality of the bromodomain with the HAT activity of coactivators in the regulation of gene transcription.

The present invention further provides both a nuclear magnetic resonance (NMR) structure of the bromodomain from the HAT coactivator P/CAF (p300/CBP-associated factor) as well as the structure for the P/CAF bromodomain in complex with acetyl-histamine. The structure reveals an unusual left-handed up-and-down four-helix bundle.

The results disclosed herein explain prior deletion experiments which showed that the bromodomain is indispensable for the function of GCN5 in yeast. Bromodomain-AcK binding also appears to be important for the assembly and activity of multiprotein complexes in transcriptional activation. The results reported herein therefore, form the foundation for identifying specific biological ligands and for defining the molecular mechanisms by which the extensive family of bromodomains participate in chromatin remodeling and transcriptional activation

As disclosed herein, the binding partner for the bromodomain is a peptide or protein comprising an acetyl-lysine (AcK). Interestingly, whereas a free acetyl-lysine does not appear to bind the bromodomain, an analog of the acetyl-lysine, acetyl-histamine, does. This is most likely due to the additional charge present in the free amino acid. Consistently, free acetyl-histidine also does not to bind the bromodomain.

The present invention further provides a key region of the bromodomain for the interaction with its acetyl-lysine binding partner, the ZA loop. The amino acid sequence of the ZA loop is defined in Figure 1 for a number of bromodomains and is depicted in Figure 2A for P/CAF. In a particular embodiment, the ZA loop has between about 21 and 40 amino acid residues comprising the amino acid sequence of :

$$F\ X_{2\text{-}3}\ P\ X_{5\text{-}8}\ J_{P/K/H}\ X\ Y\ J_{Y/F/H}\ X_5\ P\ J_{M/I/V}\ D \qquad \text{(SEQ ID NO:3)}$$

more preferably the ZA loop has about 23 to 34 amino acid residues and comprises the amino acid sequence:

$$X_2\ F\ X_{2\text{-}3}\ P\ X_{5\text{-}8}\ J_{P/K/H}\ X\ Y\ J_{Y/F/H}\ X_5\ P\ J_{M/I/V}\ D \qquad \text{(SEQ ID NO:43)}$$

(1) The single letter amino acid code is used in this description, *i.e.*,"F" for phenylalanine; "P" for proline; "Y" for tyrosine; and "D" for aspartic acid.

(2) "X" indicates any amino acid (an undesignated amino acid); and X, X_2, X_{2-3}, X_5,and X_{5-8} indicates one undesignated amino acid, two consecutive undesignated amino acids, two or three consecutive undesignated amino acids, five consecutive undesignated amino acids, and five to eight consecutive undesignated amino acids respectively.

(3) "J" indicates that identity of the amino acid is restricted to a particular group, again the one letter code is used

(i) $J_{P/K/H}$ is either proline, lysine or histidine.

(ii) $J_{Y/F/H}$ is either tyrosine, phenylalanine or histidine.

(iii) $J_{M/I/V}$ is either methionine, isoleucine, or valine.

Since this region of the bromodomain is important in binding its acetyl-lysine binding partner, antibodies specifically raised against this region are also included in the present invention. In a particular embodiment, the antibody is a humanized chimeric antibody that can be used in therapeutic treatment. Thus monoclonal, chimeric, and polyclonal antibodies raised against bromodomains, preferably against amino acid residues in the ZA loop region are part of the present invention. In a specific embodiment the antibody is raised against a peptide, fusion peptide or conjugated peptide consisting of amino acid residues 746 to 765 of SEQ ID NO:2, *i.e.*, WPFMEPVKRTEAPGYYEVIR (SEQ ID NO:44). Such antibodies can be used in the treatment of leukemia for example. Alternatively, these antibodies can be used in drug discovery assays.

Thus the present invention provides the first detailed structural information regarding a bromodomain and a bromodomain complexed with its acetylated binding partner. The present invention therefore provides the three-dimensional structure of the bromodomain and a bromodomain acetylated binding partner complex. Since the interaction of the bromodomain with a histone for example, can play a significant role in chromatin remodeling/regulation, the structural information provided herein can be employed in methods of identifying drugs that can modulate basic cell processes by modulating the transcription. In a particular embodiment, the three-dimensional

structural information is used in the design of a small organic molecule for the treatment of cancer.

Indeed, the bromodomain and lysine-acetylated protein interaction can now be implicated to play a causal role in the development of a number of diseases including cancers such as leukemia. For example, chromatin remodeling plays a central role in the etiology of viral infection and cancer [Archer and Hodin, *Curr. Opin. Genet. Biol.* **9**:171-174 (1999); Jacobson and Pillus, *Curr. Opin. Genet. Biol.* **9**:175-184 (1999)]. Both altered histone acetylation/deacetylation and aberrant forms of chromatin-remodeling complexes are associated with human diseases. Furthermore, chromosomal translocation of various cellular genes with those encoding HATs and subunits of chromatin remodeling complexes have been implicated in leukomogenesis. The *MOZ* (monocytic leukemia zinc finger) and *MLL/ALL-1* genes are frequently fused to the gene encoding the co-activator HAT CBP [Sobulo *et al.*, *Proc. Natl. Acad. Sci. USA* **94**:8732-8737(1997)]. The resulting fusion protein MLL-CBP contains the tandem bromodomain-PHD finger-HAT domain of CBP. It also has been shown that both the bromodomain and HAT domain of CBP are required for leukomogenesis, because deletion of either the bromodomain or the HAT domain results in loss of the MLL-CBP fusion protein's ability for cell transform. These results indicate that the CBP bromodomain, and more particularly, the ZA loop of the CBP bromodomain, is an excellent target for developing drugs that interfere with the bromodomain acetyl-lysine interaction that can be used in the treatment of human acute leukemia. In addition, an antibody (*e.g.*, a humanized antibody) raised specifically against a peptide from the ZA loop of the CBP bromodomain could also be effective for treating these conditions.

Furthermore, the human immunodeficiency virus type 1 (HIV-1) *trans*-activator protein, Tat, is absolutely required for productive HIV viral replication [Jeang and Gatignol, *Curr. Top. Microbiol. Immunol.*, **188**:123-144(1994)]. Recently, it has been shown that HIV-1 Tat transcriptional activity is tightly regulated by lysine acetylation [Kiernan *et al.*, *EMBO Journal* **18**:6106-6118 (1999)]. Therefore, the interaction of the acetyl-lysine of Tat with one or more bromodomain-containing proteins associated

with chromatin remodeling could mediate gene transcription. Thus, the bromodomain/lysine-acetylated Tat interaction could also serve as a drug target for blocking HIV replication in cells. Similarly, an antibody raised specifically against a peptide from the ZA loop of the bromodomain could also be effective for treating these conditions.

In addition, based on the new structural information disclosed herein, the key amino acid residues for the binding of a given bromodomain and its binding partner can be identified and further elucidated using basic mutagenesis and standard isothermal titration calorimetry, for example. In this case, both the crucial amino acids for the bromodomain and the binding partner (i.e., apart from the acetyl-lysine) can be readily determined and are also part of the present invention.

The results obtained from the structural and functional studies disclosed herein provide the foundation for both high throughput drug screening and structure-based rational drug design. The agents identified by this procedure will be useful for ameliorating conditions involving chromatin remodeling/regulation as indicated above.

Structure based rational drug design is the most efficient method of drug development. However, heretofore, no information has been disclosed regarding the structure of the bromodomain or more importantly, its interaction with the acetyl-lysine of its binding partner. Obtaining detailed structural information requires an extensive NMR or X-ray crystallographic analysis. By determining and then exploiting the detailed structural information of the bromodomain and of the bromodomain/acetyl-histamine (exemplified by NMR analysis below) the present invention provides novel methods for developing new drugs through structure based rational drug design.

Thus the present invention provides representative sets of the atomic structure coordinates of the free form of the P/CAF bromodomain (Table 5) and of the P/CAF bromodomain-acetyl-histamine complex (Table 6) which were both obtained by NMR analysis. A Ribbon diagram of the three-dimensional structure of the P/CAF bromodomain is depicted in Figure 2E, whereas the P/CAF bromodomain acetyl-lysine

binding pocket is depicted in Figure 4. The present invention also provides the NOE-derived distance restraints, and NMR chemical shift assignments of the P/CAF bromodomain. The NMR chemical shift assignments of the P/CAF bromodomain are included in the chemical shift table (Table 1) for the ^{1}H-^{15}N HSQC spectrum of P/CAF bromodomain. The unambiguous NOE-derived Inter-proton Distance Restraints (Table 2), the ambiguous NOE-derived Inter-proton Distance Restraints (Table 3) and the ^{1}H bonding restraints (Table 4) are also disclosed herein. The sample atomic coordinate data provided enable the skilled artisan to practice the invention. In addition, Tables 1-6 are also capable of being placed into a computer readable form which is also part of the present invention. Furthermore, methods of using these coordinates and chemical shifts and related information (including in computer readable forms) either individually or together in drug assays are also provided. More particularly, such atomic coordinates can be used to identify potential ligands or drugs which will modulate the binding of a bromodomain with its binding partner.

Therefore, if appearing herein, the following terms shall have the definitions set out below.

As used herein a "bromodomain-acetyl-lysine binding complex" is a binding complex between a bromodomain or fragment thereof and either a peptide/polypeptide comprising an acetyl-lysine (or an analog of acetyl-lysine), or a free analog of acetyl-lysine, such as acetyl-histamine disclosed in the Example below. Preferably, the peptide comprises at least six amino acids in addition to the acetyl-lysine. The dissociation constant of a bromodomain-acetyl-lysine binding complex is dependent on whether the lysine residue or analog thereof is acetylated or not, such that the affinity for the bromodomain and the peptide comprising the lysine residue (for example) significantly decreases when that lysine residue is not acetylated.

As used herein a "ZA loop" of a bromodomain is one protion of a bromodomain that is involved in the binding of the bromodomain to the acetyl-lysine. The structure of the ZA loop of the bromodomain of for P/CAF is depicted in Figure 2A. The ZA loop has between about 20 and 40 amino acids and comprises the amino acid sequence of SEQ ID NO:3. More preferably the ZA loop comprises between about 23 to 34 amino acids

and has the amino acid sequence SEQ ID NO:43. The amino acid sequence of the ZA loop for a representative number of individual bromodomains is shown in Figure 1.

A "polypeptide" or "peptide" comprising a fragment of a bromodomain, such as the ZA loop, or a peptide or polypeptide comprising an acetyl-lysine, as used herein can be the "fragment" alone, or a larger chimeric or fusion peptide/protein which contains the "fragment".

As used herein the terms "fusion protein" and "fusion peptide" are used interchangeably and encompass "chimeric proteins and/or chimeric peptides" and fusion "intein proteins/peptides". A fusion protein comprises at least a portion of a protein or peptide of the present invention, *e.g.*, a bromodomain, joined *via* a peptide bond to at least a portion of another protein or peptide including *e.g.*, a second bromodomain in a chimeric fusion protein. In a particular embodiment the portion of the bromodomain is antigenic. Fusion proteins can comprise a marker protein or peptide, or a protein or peptide that aids in the isolation and/or purification of the protein, for example.

As used herein, and unless otherwise specified, the terms "agent", "potential drug", "compound", "test compound" or "potential compound" are used interchangeably, and refer to chemicals which potentially have a use as an inhibitor or activator/stabilizer of bromodomain-acetyl-lysine binding. Therefore, such "agents", "potential drugs", "compounds" and "potential compounds" may be used, as described herein, in drug assays and drug screens and the like.

As used herein a "small organic molecule" is an organic compound, including a peptide [or organic compound complexed with an inorganic compound (*e.g.*, metal)] that has a molecular weight of less than 3 Kilodaltons. Such small organic molecules can be included as agents, etc. as defined above.

As used herein the term "binds to" is meant to include all such specific interactions that result in two or more molecules showing a preference for one another relative to some third molecule. This includes processes such as covalent, ionic, hydrophobic and

hydrogen bonding but does not include non-specific associations such as solvent preferences.

As used herein the term "about" signifies that a value is within twenty percent of the indicated value *i.e.*, a peptide containing "about" 20 amino acid residues can contain between 16 and 24 amino acid residues.

General Techniques for Constructing Nucleic Acids That Encode the Bromodomains and Fragments Thereof (Incuding, ZA Loops); and the Bromodomain Binding Partners of the Present Invention.

In accordance with the present invention there may be employed conventional molecular biology, microbiology, and recombinant DNA techniques within the skill of the art. Such techniques are explained fully in the literature. See, *e.g.*, Sambrook, Fritsch & Maniatis, *Molecular Cloning: A Laboratory Manual,* Second Edition (1989) Cold Spring Harbor Laboratory Press, Cold Spring Harbor, New York (herein "Sambrook *et al.*, 1989"); *DNA Cloning: A Practical Approach,* Volumes I and II (D.N. Glover ed. 1985); *Oligonucleotide Synthesis* (M.J. Gait ed. 1984); *Nucleic Acid Hybridization* [B.D. Hames & S.J. Higgins eds. (1985)]; *Transcription And Translation* [B.D. Hames & S.J. Higgins, eds. (1984)]; *Animal Cell Culture* [R.I. Freshney, ed. (1986)]; *Immobilized Cells And Enzymes* [IRL Press, (1986)]; B. Perbal, *A Practical Guide To Molecular Cloning* (1984); F.M. Ausubel *et al.* (eds.), *Current Protocols in Molecular Biology*, John Wiley & Sons, Inc. (1994).

Therefore, if appearing herein, the following terms shall have the definitions set out below.

As used herein, the term "gene" refers to an assembly of nucleotides that encode a polypeptide, and includes cDNA and genomic DNA nucleic acids.

A "vector" is a replicon, such as plasmid, phage or cosmid, to which another DNA segment may be attached so as to bring about the replication of the attached segment. A "replicon" is any genetic element (e.g., plasmid, chromosome, virus) that functions

as an autonomous unit of DNA replication *in vivo*, *i.e.*, capable of replication under its own control.

A "cassette" refers to a segment of DNA that can be inserted into a vector at specific restriction sites. The segment of DNA encodes a polypeptide of interest, and the cassette and restriction sites are designed to ensure insertion of the cassette in the proper reading frame for transcription and translation.

A cell has been "transfected" by exogenous or heterologous DNA when such DNA has been introduced inside the cell.

A "nucleic acid molecule" refers to the phosphate ester polymeric form of ribonucleosides (adenosine, guanosine, uridine or cytidine; "RNA molecules") or deoxyribonucleosides (deoxyadenosine, deoxyguanosine, deoxythymidine, or deoxycytidine; "DNA molecules"), or any phosphoester analogues thereof, such as phosphorothioates and thioesters, in either single stranded form, or a double-stranded helix. Double stranded DNA-DNA, DNA-RNA and RNA-RNA helices are possible. The term nucleic acid molecule, and in particular DNA or RNA molecule, refers only to the primary and secondary structure of the molecule, and does not limit it to any particular tertiary forms. Thus, this term includes double-stranded DNA found, *inter alia*, in linear or circular DNA molecules (*e.g.*, restriction fragments), plasmids, and chromosomes. In discussing the structure of particular double-stranded DNA molecules, sequences may be described herein according to the normal convention of giving only the sequence in the 5′ to 3′ direction along the nontranscribed strand of DNA (*i.e.*, the strand having a sequence homologous to the mRNA). A "recombinant DNA molecule" is a DNA molecule that has undergone a molecular biological manipulation.

A nucleic acid molecule is "hybridizable" to another nucleic acid molecule, such as a cDNA, genomic DNA, or RNA, when a single stranded form of the nucleic acid molecule can anneal to the other nucleic acid molecule under the appropriate conditions of temperature and solution ionic strength (*see* Sambrook *et al.*, *supra*). The conditions of temperature and ionic strength determine the "stringency" of the

hybridization. For preliminary screening for homologous nucleic acids, low stringency hybridization conditions, corresponding to a T_m of 55°, can be used, *e.g.*, 5x SSC, 0.1% SDS, 0.25% milk, and no formamide; or 30% formamide, 5x SSC, 0.5% SDS). Moderate stringency hybridization conditions correspond to a higher T_m, *e.g.*, 40% formamide, with 5x or 6x SCC. High stringency hybridization conditions correspond to the highest T_m, *e.g.*, 50% formamide, 5x or 6x SCC. Hybridization requires that the two nucleic acids contain complementary sequences, although depending on the stringency of the hybridization, mismatches between bases are possible. The appropriate stringency for hybridizing nucleic acids depends on the length of the nucleic acids and the degree of complementation, variables well known in the art. The greater the degree of similarity or homology between two nucleotide sequences, the greater the value of T_m for hybrids of nucleic acids having those sequences. The relative stability (corresponding to higher T_m) of nucleic acid hybridizations decreases in the following order: RNA:RNA, DNA:RNA, DNA:DNA. For hybrids of greater than 100 nucleotides in length, equations for calculating T_m have been derived (*see* Sambrook *et al.*, *supra*, 9.50-10.51). For hybridization with shorter nucleic acids, *i.e.*, oligonucleotides, the position of mismatches becomes more important, and the length of the oligonucleotide determines its specificity (*see* Sambrook *et al.*, *supra*, 11.7-11.8). Preferably a minimum length for a hybridizable nucleic acid is at least about 12 nucleotides; preferably at least about 18 nucleotides; and more preferably the length is at least about 27 nucleotides; and most preferably 36 nucleotides.

In a specific embodiment, the term "standard hybridization conditions" refers to a T_m of 55°C, and utilizes conditions as set forth above. In a preferred embodiment, the T_m is 60°C; in a more preferred embodiment, the T_m is 65°C.

A DNA "coding sequence" is a double-stranded DNA sequence which is transcribed and translated into a polypeptide in a cell *in vitro* or *in vivo* when placed under the control of appropriate regulatory sequences. The boundaries of the coding sequence are determined by a start codon at the 5′ (amino) terminus and a translation stop codon at the 3′ (carboxyl) terminus. A coding sequence can include, but is not limited to, prokaryotic sequences and synthetic DNA sequences. If the coding sequence is

intended for expression in a eukaryotic cell, a polyadenylation signal and transcription termination sequence will usually be located 3′ to the coding sequence.

Transcriptional and translational control sequences are DNA regulatory sequences, such as promoters, enhancers, terminators, and the like, that provide for the expression of a coding sequence in a host cell. In eukaryotic cells, polyadenylation signals are control sequences.

A "promoter sequence" is a DNA regulatory region capable of binding RNA polymerase in a cell and initiating transcription of a downstream (3′ direction) coding sequence. For purposes of defining the present invention, the promoter sequence is bounded at its 3′ terminus by the transcription initiation site and extends upstream (5′ direction) to include the minimum number of bases or elements necessary to initiate transcription at levels detectable above background. Within the promoter sequence will be found a transcription initiation site (conveniently defined for example, by mapping with nuclease S1), as well as protein binding domains (consensus sequences) responsible for the binding of RNA polymerase.

A coding sequence is "under the control" of transcriptional and translational control sequences in a cell when RNA polymerase transcribes the coding sequence into mRNA, which is then trans-RNA spliced and translated into the protein encoded by the coding sequence.

A DNA sequence is "operatively linked" to an expression control sequence when the expression control sequence controls and regulates the transcription and translation of that DNA sequence. The term "operatively linked" includes having an appropriate start signal (e.g., ATG) in front of the DNA sequence to be expressed and maintaining the correct reading frame to permit expression of the DNA sequence under the control of the expression control sequence and production of the desired product encoded by the DNA sequence. If a gene that one desires to insert into a recombinant DNA molecule does not contain an appropriate start signal, such a start signal can be inserted in front of the gene.

As used herein, the term "homologous" in all its grammatical forms refers to the relationship between proteins that possess a "common evolutionary origin," including proteins from superfamilies (*e.g.*, the immunoglobulin superfamily) and homologous proteins from different species (*e.g.*, myosin light chain, etc.) [Reeck *et al., Cell,* **50**:667 (1987)]. Such proteins have sequence homology as reflected by their high degree of sequence similarity.

Accordingly, the term "sequence similarity" in all its grammatical forms refers to the degree of identity or correspondence between nucleic acid or amino acid sequences of proteins that may or may not share a common evolutionary origin (*see* Reeck *et al.*, *supra*). However, in common usage and in the instant application, the term "homologous," when modified with an adverb such as "highly," may refer to sequence similarity and not a common evolutionary origin.

Two DNA sequences are "substantially homologous" when at least about 60% (preferably at least about 80%, and most preferably at least about 90 or 95%) of the nucleotides match over the defined length of the DNA sequences. Sequences that are substantially homologous can be identified by comparing the sequences using standard software available in sequence data banks, or in a Southern hybridization experiment under, for example, stringent conditions as defined for that particular system. Defining appropriate hybridization conditions is within the skill of the art. See, e.g., Maniatis et al., *supra*; DNA Cloning, Vols. I & II, *supra*; Nucleic Acid Hybridization, *supra*.

As used herein an amino acid sequence is 100% "homologous" to a second amino acid sequence if the two amino acid sequences are identical, and/or differ only by neutral or conservative substitutions as defined below. Accordingly, an amino acid sequence is 50% "homologous" to a second amino acid sequence if 50% of the two amino acid sequences are identical, and/or differ only by neutral or conservative substitutions.

As used herein, DNA and protein sequence percent identity can be determined using MacVector 6.0.1, Oxford Molecular Group PLC (1996) and the Clustal W algorithm with the alignment default parameters, and default parameters for identity. These

commercially available programs can also be used to determine sequence similarity using the same or analogous default parameters.

The term "corresponding to" is used herein to refer similar or homologous sequences, whether the exact position is identical or different from the molecule to which the similarity or homology is measured. Thus, the term "corresponding to" refers to the sequence similarity, and not the numbering of the amino acid residues or nucleotide bases.

As used herein a "heterologous nucleotide sequence" is a nucleotide sequence that is added to a nucleotide sequence of the present invention by recombinant methods to form a nucleic acid which is not naturally formed in nature. Such nucleic acids can encode fusion proteins or peptides, including chimeric proteins and peptides. Thus the heterologous nucleotide sequence can encode peptides and/or proteins which contain regulatory and/or structural properties. In another such embodiment the heterologous nucleotide can encode a protein or peptide that functions as a means of detecting the protein or peptide encoded by the nucleotide sequence of the present invention after the recombinant nucleic acid is expressed. In still another such embodiment the heterologous nucleotide can function as a means of detecting a nucleotide sequence of the present invention. A heterologous nucleotide sequence can comprise non-coding sequences including restriction sites, regulatory sites, promoters and the like.

The present invention also relates to cloning vectors containing nucleic acids encoding analogs and derivatives of the bromodomains of the present invention and polypeptides/peptides that can bind a bromodomain when a lysine of the polypeptide/peptide is acetylated, including modified fragments, that have the same or homologous functional activity as the individual fragments, and homologs thereof. The production and use of derivatives and analogs related to the fragments are within the scope of the present invention.

Due to the degeneracy of nucleotide coding sequences, other DNA sequences which encode substantially the same amino acid sequence as a nucleic acid encoding a protein

comprising bromodomain or bromodomain binding partner (*i.e.*, when post-transcriptionally acetylated) of the present invention for example, may be used in the practice of the present invention. These include but are not limited to allelic genes, homologous genes from other species, which are altered by the substitution of different codons that encode the same amino acid residue within the sequence, thus producing a silent change. Likewise, the peptides and polypeptides of the present invention include, but are not limited to, those containing, as a primary amino acid sequence, analogous portions of their respective amino acid sequences including altered sequences in which functionally equivalent amino acid residues are substituted for residues within the sequence resulting in a conservative amino acid substitution. For example, one or more amino acid residues within the sequence can be substituted by another amino acid of a similar polarity, which acts as a functional equivalent, resulting in a silent alteration. Substitutes for an amino acid within the sequence may be selected from other members of the class to which the amino acid belongs. For example, the nonpolar (hydrophobic) amino acids include alanine, leucine, isoleucine, valine, proline, phenylalanine, tryptophan and methionine. Amino acids containing aromatic ring structures are phenylalanine, tryptophan, and tyrosine. The polar neutral amino acids include glycine, serine, threonine, cysteine, tyrosine, asparagine, and glutamine. The positively charged (basic) amino acids include arginine, and lysine. The negatively charged (acidic) amino acids include aspartic acid and glutamic acid.

Particularly preferred conserved amino acid exchanges are:

(a) Lys for Arg or vice versa such that a positive charge may be maintained;

(b) Glu for Asp or vice versa such that a negative charge may be maintained;

(c) Ser for Thr or vice versa such that a free -OH can be maintained;

(d) Gln for Asn or vice versa such that a free NH_2 can be maintained;

(e) Ile for Leu or for Val or vice versa as roughly equivalent hydrophobic amino acids; and

(f) Phe for Tyr or vice versa as roughly equivalent aromatic amino acids.

A conservative change generally leads to less change in the structure and function of the resulting protein. A non-conservative change is more likely to alter the structure,

activity or function of the resulting protein. The present invention should be considered to include sequences containing conservative changes which do not significantly alter the activity or binding characteristics of the resulting protein. Specific amino acid residues for the P/CAF bromodomain have been identified that are important for binding, indicating a potential lower stringency for the substitution of the remaining amino acids residues.

All of the peptides/fragments of the present invention can be modified by being placed in a fusion or chimeric peptide or protein, or labeled *e.g.*, to have an N-terminal FLAG-tag, or H6 tag. In a particular embodiment the P/CAF bromodomain fragment can be modified to contain a marker protein such as green fluorescent protein as described in U.S. Patent No. 5,625,048 filed April 29, 1997 and WO 97/26333, published July 24, 1997 each of which are hereby incorporated by reference herein in their entireties.

The nucleic acids encoding peptides and protein fragments of the present invention and analogs thereof can be produced by various methods known in the art. The manipulations which result in their production can occur at the gene or protein level [Sambrook *et al.*, 1989, *supra*]. The nucleotide sequence can be cleaved at appropriate sites with restriction endonuclease(s), followed by further enzymatic modification if desired, isolated, and ligated *in vitro*. In addition a nucleic acid sequence can be mutated *in vitro* or *in vivo*, to create and/or destroy translation, initiation, and/or termination sequences, or to create variations in coding regions and/or form new restriction endonuclease sites or destroy preexisting ones, to facilitate further *in vitro* modification. Any technique for mutagenesis known in the art can be used, including but not limited to, *in vitro* site-directed mutagenesis [Hutchinson *et al.*, *J. Biol. Chem.*, **253**:6551 (1978); Zoller and Smith, *DNA*, **3**:479-488 (1984); Oliphant *et al.*, *Gene*, **44**:177 (1986); Hutchinson *et al.*, *Proc. Natl. Acad. Sci. U.S.A.*, **83**:710 (1986)], use of TAB® linkers (Pharmacia), etc. PCR techniques are preferred for site directed mutagenesis [see Higuchi, 1989, "Using PCR to Engineer DNA", in *PCR Technology: Principles and Applications for DNA Amplification*, H. Erlich, ed., Stockton Press, Chapter 6, pp. 61-70].

The identified and isolated nucleic acids can then be inserted into an appropriate cloning vector. A large number of vector-host systems known in the art may be used.

Protein expression and purification

A bacterial protein expression system can be used to make various stable isotopically labeled (^{13}C, ^{15}N, and ^{2}H) protein samples that are useful for a three-dimensional NMR structural determination of a protein complex. For example a pET14b (Novagen) bacterial expression vector can be constructed which expresses the recombinant P/CAF bromodomain as an amino-terminal His-tagged fusion protein.

Protein expression and purification can be conducted using standard procedures for His-tagged proteins [Zhou *et al.*, *J. Biol. Chem.* **270**:31119-31123 (1995)]. To optimize the level of protein expression, various bacterial growth and expression conditions can be screened, which include different *E. Coli* cell lines, and growth and protein induction temperatures. Generally, it is preferred to obtain the maximum amount of soluble protein while still inducing protein expression with a relatively low IPTG concentration *e.g.*, ~0.2mM (final concentration) at 16°C. As exemplified below, the bromodomain of P/CAF (residues 719-832 of SEQ ID NO:2 which is SEQ ID NO:7) was subcloned into the pET14b expression vector (Novagen) and expressed in *Escherichia coli* BL21(DE3) cells. Uniformly ^{15}N- and $^{15}N/^{13}C$-labeled proteins were prepared by growing bacteria in a minimal medium containing $^{15}NH_4Cl$ with or without $^{13}C_6$-glucose. A uniformly $^{15}N/^{13}C$-labeled and fractionally deuterated protein sample was prepared by growing the cells in 75% $^{2}H_2O$. The bromodomain was purified by affinity chromatography on a nickel-IDA column (Invitrogen) followed by the removal of poly-His tag by thrombin cleavage. The final purification of the protein was achieved by size-exclusion chromatography. The acetyl-lysine-containing peptides were prepared on a MilliGen 9050 peptide synthesizer (Perkin Elmer) using Fmoc/HBTU chemistry. Acetyl-lysine was incorporated using the reagent Fmoc-Ac-Lys with HBTU/DIPEA activation. NMR samples contained approximately 1 mM protein in 100mM phosphate buffer of pH 6.5 and 5mM perdeuterated DTT and 0.5mM EDTA in $H_2O/^{2}H_2O$ (9/1) or $^{2}H_2O$.

One major advantage of using the heteronuclear multidimensional approach, as exemplied herein, is that the NMR resonance assignments of a protein are obtained in a sequence-specific manner which assures accuracy and greatly facilitates data analysis and structure determination [Clore, G. M. & Gronenborn, A. M. *Meth. Enzymol.* **239**:249-363 (1994)]. In addition, the signal overlapping problems in the protein spectra are minimized by the use of multidimensional NMR spectra, which separates the proton signals according to the chemical shifts of their attached hetero-nuclei (such as ^{15}N and ^{13}C). This NMR approach has been proven very powerful for structural analysis of large proteins [Clore, G. M. & Gronenborn, A. M. *Meth. Enzymol.* **239**:249-363 (1994)]. To facilitate sequence-specific resonance assignments for the structural study, a uniformly ^{13}C, ^{15}N-labeled and fractionally (75%) deuterated protein sample of the bromodomain can be prepared by growing bacterial cells in 75% $^{2}H_2O$ as exemplified below. Such protein samples can be used for triple-resonance NMR experiments. A triple-labeled protein sample is useful for high-resolution NMR structural studies. Because of the favorable ^{1}H, ^{13}C, and ^{15}N relaxation rates caused by the partial deuteration of the protein, constant-time triple-resonance NMR spectra can be acquired with higher digital resolution and sensitivity [Sattler, M. & Fesik, S. W. *Structure* 4:1245-1249 (1996)]. In addition, various stable-isotopically labeled (^{15}N and ^{13}C /^{15}N) proteins can also be prepared using this procedure.

Synthetic Polypeptides

The term "polypeptide" is used in its broadest sense to refer to a compound of two or more subunit amino acids, amino acid analogs, or peptidomimetics. The subunits are linked by peptide bonds. The terms "polypeptide", "protein", and "peptide" are used interchangeably herein, though preferably as used herein a "peptide" refers to a compound of at least two but less than fifty subunit amino acids, and a polypeptide or protein refers to compound of fifty or more amino acids. The polypeptides of the present invention may be chemically synthesized or as detailed above, genetically engineered or isolated from natural sources.

In addition, potential drugs or agents that may be tested in the drug screening assays of the present invention may also be chemically synthesized. When the peptide is to be

modified, *e.g.*, acetylated, the modification can be at any time during the peptide synthesis, including using an acetyl-lysine as a starting material or acetylating a lysine residue of a peptide after the peptide has been synthesized. In the Example below, the acetyl-lysine-containing peptides were prepared on a MilliGen 9050 peptide synthesizer (Perkin Elmer) using Fmoc/HBTU chemistry. Acetyl-lysine was incorporated using the reagent Fmoc-Ac-Lys with HBTU/DIPEA activation.

Thus, synthetic polypeptides, prepared using the well known techniques of solid phase, liquid phase, or peptide condensation techniques, or any combination thereof, can include natural and unnatural amino acids. Amino acids used for peptide synthesis may be standard Boc (N^{α}-amino protected N^{α}-t-butyloxycarbonyl) amino acid resin with the standard deprotecting, neutralization, coupling and wash protocols of the original solid phase procedure of Merrifield [*J. Am. Chem. Soc.*, **85**:2149-2154 (1963)], or the base-labile N^{α}-amino protected 9-fluorenylmethoxycarbonyl (Fmoc) amino acids first described by Carpino and Han [*J. Org. Chem.*, **37**:3403-3409 (1972)]. Both Fmoc and Boc N^{α}-amino protected amino acids can be obtained from Fluka, Bachem, Advanced Chemtech, Sigma, Cambridge Research Biochemical, Bachem, or Peninsula Labs or other chemical companies familiar to those who practice this art. In addition, the method of the invention can be used with other N^{α}-protecting groups that are familiar to those skilled in this art. Solid phase peptide synthesis may be accomplished by techniques familiar to those in the art and provided, for example, in Stewart and Young [Solid Phase Synthesis, Second Edition, Pierce Chemical Co., Rockford, IL (1984)] and Fields and Noble [*Int. J. Pept. Protein Res.*, **35**:161-214 (1990)], or using automated synthesizers, such as sold by ABS. Thus, polypeptides of the invention may comprise D-amino acids, a combination of D- and L-amino acids, and various "designer" amino acids (*e.g.*, β-methyl amino acids, Cα-methyl amino acids, and Nα-methyl amino acids, etc.) to convey special properties. Synthetic amino acids include ornithine for lysine, fluorophenylalanine for phenylalanine, and norleucine for leucine or isoleucine. Additionally, by assigning specific amino acids at specific coupling steps, α-helices, β turns, β sheets, γ-turns, and cyclic peptides can be generated.

In a further embodiment, subunits of peptides that confer useful chemical and structural properties will be chosen. For example, peptides comprising D-amino acids will be resistant to L-amino acid-specific proteases *in vivo*. In addition, the present invention envisions preparing peptides that have more well defined structural properties, and the use of peptidomimetics, and peptidomimetic bonds, such as ester bonds, to prepare peptides with novel properties. In another embodiment, a peptide may be generated that incorporates a reduced peptide bond, i.e., R_1-**CH_2-NH**-R_2, where R_1 and R_2 are amino acid residues or sequences. A reduced peptide bond may be introduced as a dipeptide subunit. Such a molecule would be resistant to peptide bond hydrolysis, *e.g.*, protease activity. Such peptides would provide ligands with unique function and activity, such as extended half-lives *in vivo* due to resistance to metabolic breakdown, or protease activity. Furthermore, it is well known that in certain systems constrained peptides show enhanced functional activity [Hruby, *Life Sciences,* **31**:189-199 (1982); Hruby *et al.*, *Biochem J.,* **268**:249-262 (1990)]; the present invention provides a method to produce a constrained peptide that incorporates random sequences at all other positions.

Constrained and cyclic peptides. A constrained, cyclic or rigidized peptide may be prepared synthetically, provided that in at least two positions in the sequence of the peptide an amino acid or amino acid analog is inserted that provides a chemical functional group capable of crosslinking to constrain, cyclise or rigidize the peptide after treatment to form the crosslink. Cyclization will be favored when a turn-inducing amino acid is incorporated. Examples of amino acids capable of crosslinking a peptide are cysteine to form disulfides, aspartic acid to form a lactone or a lactam, and a chelator such as γ-carboxyl-glutamic acid (Gla) (Bachem) to chelate a transition metal and form a cross-link. Protected γ-carboxyl glutamic acid may be prepared by modifying the synthesis described by Zee-Cheng and Olson [*Biophys. Biochem. Res. Commun.,* **94**:1128-1132 (1980)]. A peptide in which the peptide sequence comprises at least two amino acids capable of crosslinking may be treated, *e.g.*, by oxidation of cysteine residues to form a disulfide or addition of a metal ion to form a chelate, so as to crosslink the peptide and form a constrained, cyclic or rigidized peptide.

The present invention provides strategies to systematically prepare cross-links. For example, if four cysteine residues are incorporated in the peptide sequence, different protecting groups may be used (Hiskey, in The Peptides: Analysis, Synthesis, Biology, Vol. 3, Gross and Meienhofer, eds., Academic Press: New York, pp. 137-167 (1981); Ponsanti *et al.*, *Tetrahedron,* **46**:8255-8266 (1990)]. The first pair of cysteines may be deprotected and oxidized, then the second set may be deprotected and oxidized. In this way a defined set of disulfide cross-links may be formed. Alternatively, a pair of cysteines and a pair of chelating amino acid analogs may be incorporated so that the cross-links are of a different chemical nature.

Non-classical amino acids that induce conformational constraints. The following non-classical amino acids may be incorporated in the peptide in order to introduce particular conformational motifs: 1,2,3,4-tetrahydroisoquinoline-3-carboxylate [Kazmierski *et al.*, *J. Am. Chem. Soc.*, **113**:2275-2283 (1991)]; (2S,3S)-methyl-phenylalanine, (2S,3R)-methyl-phenylalanine, (2R,3S)-methyl-phenylalanine and (2R,3R)-methyl-phenylalanine (Kazmierski and Hruby, *Tetrahedron Lett.* (1991)]; 2-aminotetrahydronaphthalene-2-carboxylic acid [Landis, Ph.D. Thesis, University of Arizona (1989)]; hydroxy-1,2,3,4-tetrahydroisoquinoline-3-carboxylate [Miyake *et al.*, *J. Takeda Res. Labs.*, **43**:53-76 (1989)]; β-carboline (D and L) [Kazmierski, Ph.D. Thesis, University of Arizona (1988)]; HIC (histidine isoquinoline carboxylic acid) [Zechel *et al.*, *Int. J. Pep. Protein Res.*, 43 (1991)]; and HIC (histidine cyclic urea) (Dharanipragada).

The following amino acid analogs and peptidomimetics may be incorporated into a peptide to induce or favor specific secondary structures: LL-Acp (LL-3-amino-2-propenidone-6-carboxylic acid), a β-turn inducing dipeptide analog [Kemp *et al.*, *J. Org. Chem.*, **50**:5834-5838 (1985)]; β-sheet inducing analogs [Kemp *et al.*, *Tetrahedron Lett.*, **29**:5081-5082 (1988); β-turn inducing analogs [Kemp *et al.*, *Tetrahedron Lett.*, **29**:5057-5060 (1988)]; ∝-helix inducing analogs (Kemp *et al.*, *Tetrahedron Lett.*, **29**:4935-4938 (1988)]; γ-turn inducing analogs [Kemp *et al.*, *J. Org. Chem.*, **54**:109:115 (1989)]; and analogs provided by the following references: Nagai and Sato, *Tetrahedron Lett.*, **26**:647-650 (1985); DiMaio *et al.*, *J. Chem. Soc. Perkin Trans.*, p. 1687 (1989); also a Gly-Ala turn analog [Kahn *et al.*, *Tetrahedron*

spectra of mutated proteins can be compared to that of the wild-type protein bromodomain.

Chemical-shift perturbations due to ligand binding have proven to be a reliable and sensitive probe for the ligand binding site of the protein. This is because the chemical-shift changes of the backbone amide groups are likely to reflect any changes in protein conformation and/or hydrogen bonding due to the peptide/ligand binding. To examine the effects of a mutation on the ligand binding (in this case the ligand is a peptide comprising an acetyl-lysine), peptide titration experiments can be conducted by following the changes of $^{1}H/^{15}N$ signals of the mutant proteins as a function of the peptide concentration. These experiments indicate whether the acetyl-lysine binding site remains the same or changes in the mutants relative to the wild type protein. The effects of the mutation on the peptide binding affinity can also be examined by NMR spectroscopy. If the mutated proteins result in the reduction of the binding affinity, a change of the exchange phenomenon between the free and the ligand-bound signals should be observed in NMR spectrum. If the reduction in binding affinity causes the peptide binding to change from a slow exchange rate to a fast exchange rate, on the NMR time scale, then the peptide binding affinity can be determined from the NMR titration experiment. From these mutation analyses key amino acid residues that are important for binding a peptide comprising the acetyl-lysine can be identified. Such analysis has been exemplified below.

Protein Structure Determination by NMR Spectroscopy

The NMR results from the present invention are summarized by the atomic structure coordinates of the free form of the P/CAF bromodomain (Table 5) and of the P/CAF bromodomain-acetyl-histamine complex (Table 6). The NMR chemical shift assignments of the P/CAF bromodomain are included in the chemical shift table (Table 1) for the ^{1}H-^{15}N HSQC spectrum of P/CAF bromodomain. The unambiguous NOE-derived Inter-proton Distance Restraints are in Table 2, the ambiguous NOE-derived Inter-proton Distance Restraints are in Table 3, and the ^{1}H bonding restraints are disclosed in Table 4.

Backbone and Side-chain Assignments: Sequence-specific backbone assignment can be achieved by using a suite of deuterium-decoupled triple-resonance 3D NMR experiments which include HNCA, HN(CO)CA, HN(CA)CB, HN(COCA)CB, HNCO, and HN(CA)CO experiments [Yamazaki, *et al.*, *J. Am. Chem. Soc.* **116**:11655-11666 (1994)]. The water flip-back scheme is used in these NMR pulse programs to minimize amide signal attenuation from water exchange. Sequential side-chain assignments are typically accomplished from a series of 3D NMR experiments with alternative approaches to confirm the assignments. These experiments include 3D ^{15}N TOCSY-HSQC, HCCH-TOCSY, (H)C(CO)NH-TOCSY, and H(C)(CO)NH-TOCSY [*see* Clore, G. M. & Gronenborn, A. M. *Meth. Enzymol.* **239**:249-363 (1994);Sattler *et al.*, *Prog. in Nuclear Magnetic Resonance Spec.* **4**:93-158 (1999)].

Stereospecific Methyl Groups: Stereospecific assignments of methyl groups of Valine and Leucine residues can be obtained from an analysis of carbon signal multiplet splitting using a fractionally ^{13}C-labeled protein sample, which can be readily prepared using M9 minimal medium containing 10% ^{13}C-/90%^{12}C-glucose mixture [*see* Neri, *et al.*, *Biochemistry* **28**:7510-7516 (1989)].

Dihedral Angle Restraints: Backbone dihedral angle (Φ) constraints can be generated from the $^{3}J_{HNH\alpha}$ coupling constants measured in a HNHA-*J* experiment [*see* Vuister, G. & Bax, A. *J. Am. Chem. Soc.* **115**:7772-7777 (1993)]. Side-chain dihedral angles ($\chi 1$) can be obtained from short mixing time ^{15}N-edited 3D TOCSY-HSQC [*see* Clore, *et al.*, *J. Biomol. NMR* **1**:13-22 (1991)] and 3D HNHB experiments [*see* Matson *et al.*, *J. Biomol. NMR* **3**:239-244 (1993)], which can also provide stereospecific assignments of β methylene protons.

Hydrogen Bonds Restraints: Amide protons that are involved in hydrogen bonds can be identified from an analysis of amide exchange rates measured from a series of 2D $^{1}H/^{15}N$ HSQC spectra recorded after adding $^{2}H_2O$ to the protein sample.

NOE Distance Restraints: Distance restraints are obtained from analysis of ^{15}N, and ^{13}C-edited 3D NOESY data, which can be collected with different mixing times to minimize spin diffusion problems. The nuclear Overhauser effect (NOE)-derived

restraints are categorized as strong (1.8-3 Å), medium (1.8-4 Å) or weak (1.8-5 Å) based on the observed NOE intensities. A recently developed procedure for the iterative automated NOE analysis by using ARIA [*see* Nilges *et al.*, *Prog. NMR Spectroscopy* **32**:107-139 (1998)] can be employed which integrates with X-PLOR for structural calculations. To ensure the success of ARIA/X-PLOR-assisted NOE analysis and structure calculations, the ARIA assigned NOE peaks can be manually confirmed.

Intermolecular NOE Distance Restrains: For the structural determination of a protein/peptide complex, intermolecular NOE distance restraints can be obtained from a ^{13}C-edited (F_1) and ^{15}N, and ^{13}C-filtered (F_3) 3D NOESY data set collected for a sample containing isotope-labeled protein and non-labeled peptide.

Structure Calculations and Refinements: Structures of the protein can be generated using a distance geometry/simulated annealing protocol with the X-PLOR program [*see* Nilges,*et al.*, *FEBS Lett.* **229**:317-324 (1988); Kuszewski, *et al.*, *J. Biolmol. NMR* **2**:33-56 (1992); Brünger, A. T. *X-PLOR Version 3.1: A system for X-Ray crystallography and NMR* (Yale University Press, New Haven, CT, 1993)]. The structure calculations can employ inter-proton distance restraints obtained from ^{15}N- and ^{13}C-resolved NOESY spectra. The initial low-resolution structures can be used to facilitate NOE assignments, and help identify hydrogen bonding partners for slowly exchanging amide protons. The experimental restraints of dihedral angles and hydrogen bonds can be included in the distance restraints for structure refinements.

Protein-Structure Based Design of Agonists and Antagonists of the Bromodomain-Acetyl-Lysine Binding Complex

Once the three-dimensional structure of the Bromodomain and the Bromodomain-acetyl-lysine binding complex are determined, a potential drug or agent (antagonist or agonist) can be examined through the use of computer modeling using a docking program such as GRAM, DOCK, or AUTODOCK [Dunbrack *et al.*, 1997, *supra*]. This procedure can include computer fitting of potential agents to the bromodomain, for example, to ascertain how well the shape and the chemical structure of the potential ligand will complement or interfere with the interaction between the bromodomain and

the acetyl-lysine [Bugg *et al.*, *Scientific American*, **Dec.**:92-98 (1993); West *et al.*, *TIPS*, **16**:67-74 (1995)]. Computer programs can also be employed to estimate the attraction, repulsion, and steric hindrance of the agent to the dimer-dimer binding site, for example. Generally the tighter the fit (*e.g.*, the lower the steric hindrance, and/or the greater the attractive force) the more potent the potential drug will be since these properties are consistent with a tighter binding constant. Furthermore, the more specificity in the design of a potential drug the more likely that the drug will not interfere with related proteins. This will minimize potential side-effects due to unwanted interactions with other proteins.

Initially a potential drug could be obtained by screening a random peptide library produced by recombinant bacteriophage for example, [Scott and Smith, *Science,* **249**:386-390 (1990); Cwirla *et al.*, *Proc. Natl. Acad. Sci.*, **87**:6378-6382 (1990); Devlin *et al.*, *Science,* **249**:404-406 (1990)] or a chemical library. An agent selected in this manner could be then be systematically modified by computer modeling programs until one or more promising potential drugs are identified. Such analysis has been shown to be effective in the development of HIV protease inhibitors [Lam *et al.*, *Science* **263**:380-384 (1994); Wlodawer *et al.*, *Ann. Rev. Biochem.* **62**:543-585 (1993); Appelt, *Perspectives in Drug Discovery and Design* **1**:23-48 (1993); Erickson, *Perspectives in Drug Discovery and Design* **1**:109-128 (1993)].

Such computer modeling allows the selection of a finite number of rational chemical modifications, as opposed to the countless number of essentially random chemical modifications that could be made, any one of which might lead to a useful drug. Each chemical modification requires additional chemical steps, which while being reasonable for the synthesis of a finite number of compounds, quickly becomes overwhelming if all possible modifications needed to be synthesized. Thus, through the use of the three-dimensional structural analysis disclosed herein and computer modeling, a large number of these compounds can be rapidly screened on the computer monitor screen, and a few likely candidates can be determined without the laborious synthesis of untold numbers of compounds.

Once a potential drug (agonist or antagonist) is identified it can be either selected from a library of chemicals as are commercially available from most large chemical companies including Merck, GlaxoWelcome, Bristol Meyers Squib, Monsanto/Searle, Eli Lilly, Novartis and Pharmacia UpJohn, or alternatively the potential drug may be synthesized *de novo*. As mentioned above, the *de novo* synthesis of one or even a relatively small group of specific compounds is reasonable in the art of drug design.

The potential drug can then be tested in any standard binding assay (including in high throughput binding assays) for its ability to bind to the ZA loop of a bromodomain. Alternatively the potential drug can be tested for its ability to modulate the binding of a bromodomain to acetylated histamine, for example. When a suitable potential drug is identified, a second NMR structural analysis can optionally be performed on the binding complex formed between the bromodomain-acetyl-lysine binding complex, or the bromodomain alone and the potential drug. Computer programs that can be used to aid in solving such three-dimensional structures include QUANTA, CHARMM, INSIGHT, SYBYL, MACROMODE, and ICM, MOLMOL, RASMOL, AND GRASP [Kraulis, *J. Appl Crystallogr.* **24**:946-950 (1991)]. Most if not all of these programs and others as well can be also obtained from the WorldWideWeb through the internet.

Using the approach described herein and equipped with the structural analysis disclosed herein, the three-dimensional structures of other bromodomain-acetyl-lysine binding complexes can more readily be obtained and analyzed. Such analysis will, in turn, allow corresponding drug screening methodology to be performed using the three-dimensional structures of such related complexes.

For all of the drug screening assays described herein further refinements to the structure of the drug will generally be necessary and can be made by the successive iterations of any and/or all of the steps provided by the particular drug screening assay, including further structural analysis by NMR, for example.

Phage libraries for Drug Screening.

Phage libraries have been constructed which when infected into host *E. coli* produce random peptide sequences of approximately 10 to 15 amino acids [Parmley and Smith,

Gene **73**:305-318 (1988), Scott and Smith, Science **249**:386-249 (1990)]. Specifically, the phage library can be mixed in low dilutions with permissive *E. coli* in low melting point LB agar which is then poured on top of LB agar plates. After incubating the plates at 37°C for a period of time, small clear plaques in a lawn of *E. coli* will form which represents active phage growth and lysis of the *E. coli*. A representative of these phages can be absorbed to nylon filters by placing dry filters onto the agar plates. The filters can be marked for orientation, removed, and placed in washing solutions to block any remaining absorbent sites. The filters can then be placed in a solution containing, for example, a radioactive bromodomain. After a specified incubation period, the filters can be thoroughly washed and developed for autoradiography. Plaques containing the phage that bind to the radioactive bromodomain can then be identified. These phages can be further cloned and then retested for their ability to bind to the bromodomain as before. Once the phage has been purified, the binding sequence contained within the phage can be determined by standard DNA sequencing techniques. Once the DNA sequence is known, synthetic peptides can be generated which are encoded by these sequences. These peptides can be tested, for example, for their ability to modulate the affinity of the bromodomain for its binding partner (*e.g.*, a protein comprising an acetyl-lysine or a fragment of that protein).

The effective peptide(s) can be synthesized in large quantities for use in *in vivo* models and eventually in humans to treat certain tumors. It should be emphasized that synthetic peptide production is relatively non-labor intensive, easily manufactured, quality controlled and thus, large quantities of the desired product can be produced quite cheaply. Similar combinations of mass produced synthetic peptides have been used with great success [Patarroyo, *Vaccine,* **10**:175-178 (1990)].

Drug Screening Assays

The drug screening assays of the present invention may use any of a number of means for determining the interaction between an agent or drug and a peptide comprising an acetyl-lysine and/or a bromodomain. Thus, standard high throughput drug screening procedures can be employed using a library of low molecular weight compounds, for

example that can be screened to identify a binding partner for the bromodoamin. Any such chemical library can be used including those discussed above.

In a particular assay, a bromodomain is placed on or coated onto a solid support. Methods for placing the peptides or proteins on the solid support are well known in the art and include such things as linking biotin to the protein and linking avidin to the solid support. An agent is allowed to equilibrate with the bromodomain to test for binding. Generally, the solid support is washed and agents that are retained are selected as potential drugs. Alternatively, a peptide comprising an acetyl-lysine is placed on or coated onto a solid support. In a particular embodiment of this type, the peptide comprises the amino acid sequence of SEQ ID NO:4.

The agent may be labeled. For example, in one embodiment radiolabeled agents are used to measure the binding of the agent. In another embodiment the agents have fluorescent markers. In yet another embodiment, a Biocore chip (Pharmacia) coated with the bromodomain is used, for example and the change in surface conductivity can be measured.

In addition, since a number of proteins have been identified that contain bromodomains, and the binding partners of many of these proteins are known, the fact that the bromodomain specifically binds to an acetylated lysine as disclosed herein allows the identification and preparation of a number of potential modulators of the bromodomain-acetyl-lysine binding complex based on the amino acid sequences of the binding partners to the proteins. Such potential modulators include : ISYGR-*AcK*-KRRQRR (SEQ ID NO:4), ARKSTGG-A*cK*-APRKQL (SEQ ID NO:5) and QSTSRHK-*AcK*-LMFKTE (SEQ ID NO:6) which bind to the P/CAF bromodomain as shown in the Example, below. Such peptides also can be used, for example, as a starting point for the design of an inhibitor of the bromodomain-acetyl-lysine binding complex.

Alternatively, a drug can be specifically designed to bind to the ZA loop of a bromodomain for example, such as the P/CAF bromodomain, and be assayed through NMR based methodology [Shuker *et al.*, *Science* **274**:1531-1534 (1996) hereby

incorporated by reference in its entirety.] In a particular embodiment, analogs of the binding partner of the bromodomain can be used in this analysis. One such peptide has the amino acid sequence of SEQ ID NO:4. In another embodiment of this type, the peptide has the amino acid sequence of SEQ ID NO:5. In another such embodiment of this type, the peptide has the amino acid sequence of SEQ ID NO:6.

The assay begins with contacting a compound with a ^{15}N-labeled bromodomain. Binding of the compound with the ZA loop of the bromodomain can be determined by monitoring the ^{15}N- or ^{1}H-amide chemical shift changes in two dimensional ^{15}N-heteronuclear single-quantum correlation (^{15}N-HSQC) spectra upon the addition of the compound to the ^{15}N-labeled bromodomain. Since these spectra can be rapidly obtained, it is feasible to screen a large number of compounds [Shuker *et al.*, *Science* **274**:1531-1534 (1996)]. A compound is identified as a potential ligand if it binds to the ZA loop of the bromodomain. In a further embodiment, the potential ligand can then be used as a model structure, and analogs to the compound can be obtained (e.g, from the vast chemical libraries commercially available, or alternatively through *de novo* synthesis). The analogs are then screened for their ability to bind the ZA loop of the bromodomain thus to obtain a ligand. An analog of the potential ligand is chosen as a ligand when it binds to the ZA loop of the bromodomain with a higher binding affinity than the potential ligand. In a preferred embodiment of this type the analogs are screened by monitoring the ^{15}N- or ^{1}H-amide chemical shift changes in two dimensional ^{15}N-heteronuclear single-quantum correlation (^{15}N-HSQC) spectra upon the addition of the analog to the ^{15}N-labeled bromodomain as described above.

In another further embodiment, compounds are screened for binding to two nearby sites on the bromodomain. In this case, a compound that binds a first site of the bromodomain does not bind a second nearby site. Binding to the second site can be determined by monitoring changes in a different set of amide chemical shifts in either the original screen or a second screen conducted in the presence of a ligand (or potential ligand) for the first site. From an analysis of the chemical shift changes the approximate location of a potential ligand for the second site is identified. Optimization of the second ligand for binding to the site is then carried out by screening structurally related compounds (*e.g.*, analogs as described above). When

ligands for the first site and the second site are identified, their location and orientation in the ternary complex can be determined experimentally either by NMR spectroscopy or X-ray crystallography. On the basis of this structural information, a linked compound is synthesized in which the ligand for the first site and the ligand for the second site are linked. In a preferred embodiment of this type the two ligands are covalently linked. This linked compound is tested to determine if it has a higher binding affinity for the bromodomain than either of the two individual ligands. A linked compound is selected as a ligand when it has a higher binding affinity for the bromodomain than either of the two ligands. In a preferred embodiment the affinity of the linked compound with the bromodomain is determined monitoring the ^{15}N- or ^{1}H-amide chemical shift changes in two dimensional ^{15}N-heteronuclear single-quantum correlation (^{15}N-HSQC) spectra upon the addition of the linked compound to the ^{15}N-labeled bromodomain as described above.

A larger linked compound can be constructed in an analogous manner, *e.g.*, linking three ligands which bind to three nearby sites on the bromodomain to form a multilinked compound that has an even higher affinity for the bromodomain than the linked compound.

Identification of New Bromodomains

By disclosing that protein bound acetyl-lysine is a binding partner for bromodomains, the present invention provides a method of identifying novel proteins that contain bromodomains. In short, a protein fragment or analog thereof comprising an acetyl-lysine can be used as bait to identify a binding partner that comprises a bromodomain. Any one of a number of procedures can be carried out to identify such a binding partner. One such assay comprises passing a cell extract over the bait peptide which is attached to a solid support. After washing the solid support to remove any non-specific binders, the bromodomain containing protein can be eluted from the solid support with an appropriate eluant. In a particular embodiment, the free bait peptide can be used in the elution. Other methodology includes the use of a yeast two-hybrid system, a GST pull down assay, ELISA, immunometric assays, and a modification of the CORT procedure of Schlessinger *et al.*, (US Patent No. 5,858,686, Issued on

January 12, 1999 which is hereby incorporated by reference in its entirety) for use with the bromodomain-acetyl-lysine binding complex.

Labels:

Suitable labels include enzymes, fluorophores (*e.g.*, fluorescein isothiocyanate (FITC), phycoerythrin (PE), Texas red (TR), rhodamine, free or chelated lanthanide series salts, especially Eu^{3+}, to name a few fluorophores), chromophores, radioisotopes, chelating agents, dyes, colloidal gold, latex particles, ligands (*e.g.*, biotin), and chemiluminescent agents. When a control marker is employed, the same or different labels may be used for the test and control marker gene.

In the instance where a radioactive label, such as the isotopes ^{3}H, ^{14}C, ^{32}P, ^{35}S, ^{36}Cl, ^{51}Cr, ^{57}Co, ^{58}Co, ^{59}Fe, ^{90}Y, ^{125}I, ^{131}I, and ^{186}Re are used, known currently available counting procedures may be utilized. In the instance where the label is an enzyme, detection may be accomplished by any of the presently utilized colorimetric, spectrophotometric, fluorospectrophotometric, amperometric or gasometric techniques known in the art.

Direct labels are one example of labels which can be used according to the present invention. A direct label has been defined as an entity, which in its natural state, is readily visible, either to the naked eye, or with the aid of an optical filter and/or applied stimulation, e.g. U.V. light to promote fluorescence. Among examples of colored labels, which can be used according to the present invention, include metallic sol particles, for example, gold sol particles such as those described by Leuvering (U.S. Patent 4,313,734); dye sole particles such as described by Gribnau *et al.* (U.S. Patent 4,373,932 and May *et al.* (WO 88/08534); dyed latex such as described by May, *supra*, Snyder (EP-A 0 280 559 and 0 281 327); or dyes encapsulated in liposomes as described by Campbell et al. (U.S. Patent 4,703,017). Other direct labels include a radionucleotide, a fluorescent moiety or a luminescent moiety. In addition to these direct labeling devices, indirect labels comprising enzymes can also be used according to the present invention. Various types of enzyme linked immunoassays are well known in the art, for example, alkaline phosphatase and horseradish peroxidase,

lysozyme, glucose-6-phosphate dehydrogenase, lactate dehydrogenase, urease, these and others have been discussed in detail by Eva Engvall in Enzyme Immunoassay ELISA and EMIT in *Methods in Enzymology*, **70**:419-439 (1980) and in U.S. Patent 4,857,453.

Suitable enzymes include, but are not limited to, alkaline phosphatase, β-galactosidase, green fluorescent protein and its derivatives, luciferase, and horseradish peroxidase.

Other labels for use in the invention include magnetic beads or magnetic resonance imaging labels.

Antibodies to Portions of the Bromodomain that Interact with Acetyl-Lysine

According to the present invention, the bromodomains, and more particularly the ZA loops of the bromodomains and fragments thereof can be produced by a recombinant source, or through chemical synthesis, or through the modification of these peptides and fragments; and derivatives or analogs thereof, including fusion proteins, may be used as an immunogen to generate antibodies that specifically interfere with the formation of the bromodomain-acetyl-lysine binding complex. Similarly, antibodies can be raised against peptides that comprise one or more acetyl-lysine residues which also interfere with the formation of the bromodomain-acetyl-lysine binding complex. Such antibodies include but are not limited to polyclonal, monoclonal, chimeric, single chain, Fab fragments, and a Fab expression library.

Various procedures known in the art may be used for the production of the polyclonal antibodies. For the production of antibody, various host animals can be immunized by injection with the peptide having the amino acid sequence of SEQ ID NO:3, for example, or a derivative (*e.g.*, or fusion protein) thereof, including but not limited to rabbits, mice, rats, sheep, goats, etc. In one embodiment, the peptide can be conjugated to an immunogenic carrier, *e.g.*, bovine serum albumin (BSA) or keyhole limpet hemocyanin (KLH). Various adjuvants may be used to increase the immunological response, depending on the host species, including but not limited to Freund's (complete and incomplete), mineral gels such as aluminum hydroxide, surface

active substances such as lysolecithin, pluronic polyols, polyanions, peptides, oil emulsions, keyhole limpet hemocyanins, dinitrophenol, and potentially useful human adjuvants such as BCG (*bacille Calmette-Guerin*) and *Corynebacterium parvum*.

For preparation of monoclonal antibodies directed toward the peptides or protein fragments of the present invention, or analog, or derivative thereof, any technique that provides for the production of antibody molecules by continuous cell lines in culture may be used. These include but are not limited to the hybridoma technique originally developed by Kohler and Milstein [*Nature,* **256**:495-497 (1975)], as well as the trioma technique, the human B-cell hybridoma technique [Kozbor *et al., Immunology Today,* **4**:72 (1983); Cote *et al., Proc. Natl. Acad. Sci. U.S.A.,* **80**:2026-2030 (1983)], and the EBV-hybridoma technique to produce human monoclonal antibodies [Cole *et al.,* in *Monoclonal Antibodies and Cancer Therapy*, Alan R. Liss, Inc., pp. 77-96 (1985)]. In an additional embodiment of the invention, monoclonal antibodies can be produced in germ-free animals utilizing technology described in PCT/US90/02545. In fact, according to the invention, techniques developed for the production of "chimeric antibodies" [Morrison *et al., J. Bacteriol.*, **159**:870 (1984); Neuberger *et al., Nature,* **312**:604-608 (1984); Takeda *et al.*, *Nature,* **314**:452-454 (1985)] by splicing the genes from a mouse antibody molecule specific for the peptide having the amino acid sequence of SEQ ID NO:3, for example, together with genes from a human antibody molecule of appropriate biological activity can be used; such antibodies are within the scope of this invention. Such human or humanized chimeric antibodies are preferred for use in therapy of human diseases or disorders (described *infra*), since the human or humanized antibodies are much less likely than xenogenic antibodies to induce an immune response, in particular an allergic response, themselves.

According to the invention, techniques described for the production of single chain antibodies [U.S. Patent Nos. 5,476,786 and 5,132,405 to Huston; U.S. Patent 4,946,778] can be adapted to produce specific single chain antibodies. An additional embodiment of the invention utilizes the techniques described for the construction of Fab expression libraries [Huse *et al., Science,* **246**:1275-1281 (1989)] to allow rapid and easy identification of monoclonal Fab fragments with the desired specificity.

Antibody fragments which contain the idiotype of the antibody molecule can be generated by known techniques. For example, such fragments include but are not limited to: the $F(ab')_2$ fragment which can be produced by pepsin digestion of the antibody molecule; the Fab' fragments which can be generated by reducing the disulfide bridges of the $F(ab')_2$ fragment, and the Fab fragments which can be generated by treating the antibody molecule with papain and a reducing agent.

In the production of antibodies, screening for the desired antibody can be accomplished by techniques known in the art, *e.g.*, radioimmunoassay, ELISA (enzyme-linked immunosorbant assay), "sandwich" immunoassays, immunoradiometric assays, gel diffusion precipitin reactions, immunodiffusion assays, *in situ* immunoassays (using colloidal gold, enzyme or radioisotope labels, for example), western blots, precipitation reactions, agglutination assays (*e.g.*, gel agglutination assays, hemagglutination assays), complement fixation assays, immunofluorescence assays, protein A assays, and immunoelectrophoresis assays, etc. In one embodiment, antibody binding is detected by detecting a label on the primary antibody. In another embodiment, the primary antibody is detected by detecting binding of a secondary antibody or reagent to the primary antibody. In a further embodiment, the secondary antibody is labeled. Many means are known in the art for detecting binding in an immunoassay and are within the scope of the present invention. For example, to select antibodies which recognize a specific epitope of a ZA loop of a bromodomain, for example, one may assay generated hybridomas for a product which binds to a bromodomain fragment containing such an epitope and choose those which do not cross-react with bromodomain fragments that do not include that epitope.

In a specific embodiment, antibodies that interfere with the formation of the bromodomain-acetyl-lysine complex can be generated. Such antibodies can be tested using the assays described and could potentially be used in anti-cancer therapies.

Administration

According to the invention, the component or components of a therapeutic composition, *e.g.*, an agent of the invention that interferes with the bromodomain-

acetyl-lysine binding complex such as the peptide having the amino acid sequence of SEQ ID NOs:4, 5, or 6 and a pharmaceutically acceptable carrier, may be introduced parenterally, transmucosally, *e.g.*, orally, nasally, or rectally, or transdermally. Preferably, administration is parenteral, *e.g.*, via intravenous injection, and also including, but is not limited to, intra-arteriole, intramuscular, intradermal, subcutaneous, intraperitoneal, intraventricular, and intracranial administration.

In a preferred aspect, the agent of the present invention can cross cellular and nuclear membranes, which would allow for intravenous or oral administration. Strategies are available for such crossing, including but not limited to, increasing the hydrophobic nature of a molecule; introducing the molecule as a conjugate to a carrier, such as a ligand to a specific receptor, targeted to a receptor; and the like.

The present invention also provides for conjugating targeting molecules to such an agent. "Targeting molecule" as used herein shall mean a molecule which, when administered *in vivo*, localizes to desired location(s). In various embodiments, the targeting molecule can be a peptide or protein, antibody, lectin, carbohydrate, or steroid. In one embodiment, the targeting molecule is a peptide ligand of a receptor on the target cell. In a specific embodiment, the targeting molecule is an antibody. Preferably, the targeting molecule is a monoclonal antibody. In one embodiment, to facilitate crosslinking the antibody can be reduced to two heavy and light chain heterodimers, or the $F(ab')_2$ fragment can be reduced, and crosslinked to the agent via the reduced sulfhydryl. Antibodies for use as targeting molecule are specific for a cell surface antigen.

In another embodiment, the therapeutic compound can be delivered in a vesicle, in particular a liposome [*see* Langer, *Science,* **249**:1527-1533 (1990); Treat *et al.*, in *Liposomes in the Therapy of Infectious Disease and Cancer*, Lopez-Berestein and Fidler (eds.), Liss: New York, pp. 353-365 (1989); Lopez-Berestein, *ibid.*, pp. 317-327; see generally *ibid.*].

In yet another embodiment, the therapeutic compound can be delivered in a controlled release system. For example, the agent may be administered using intravenous

infusion, an implantable osmotic pump, a transdermal patch, liposomes, or other modes of administration. In one embodiment, a pump may be used [*see* Langer, *supra*; Sefton, *CRC Crit. Ref. Biomed. Eng.*, **14**:201 (1987); Buchwald *et al.*, *Surgery*, **88**:507 (1980); Saudek *et al.*, *N. Engl. J. Med.*, **321**:574 (1989)]. In another embodiment, polymeric materials can be used [*see Medical Applications of Controlled Release*, Langer and Wise (eds.), CRC Press: Boca Raton, Florida (1974); *Controlled Drug Bioavailability, Drug Product Design and Performance*, Smolen and Ball (eds.), Wiley: New York (1984); Ranger and Peppas, *J. Macromol. Sci. Rev. Macromol. Chem.*, **23**:61 (1983); see also Levy *et al.*, *Science*, **228**:190 (1985); During *et al.*, *Ann. Neurol.*, **25**:351 (1989); Howard *et al.*, *J. Neurosurg.*, **71**:105 (1989)]. In yet another embodiment, a controlled release system can be placed in proximity of the therapeutic target, *i.e.*, the bone marrow, thus requiring only a fraction of the systemic dose [*see, e.g.*, Goodson, in *Medical Applications of Controlled Release*, *supra*, vol. 2, pp. 115-138 (1984)]. Other controlled release systems are discussed in the review by Langer [*Science*, **249**:1527-1533 (1990)].

Pharmaceutical Compositions. In yet another aspect of the present invention, provided are pharmaceutical compositions of the above. Such pharmaceutical compositions may be for administration for injection, or for oral, pulmonary, nasal or other forms of administration. In general, comprehended by the invention are pharmaceutical compositions comprising effective amounts of a low molecular weight component or components, or derivative products, of the invention together with pharmaceutically acceptable diluents, preservatives, solubilizers, emulsifiers, adjuvants and/or carriers. Such compositions include diluents of various buffer content (*e.g.*, Tris-HCl, acetate, phosphate), pH and ionic strength; additives such as detergents and solubilizing agents (*e.g.*, Tween 80, Polysorbate 80), anti-oxidants (*e.g.*, ascorbic acid, sodium metabisulfite), preservatives (*e.g.*, Thimersol, benzyl alcohol) and bulking substances (*e.g.*, lactose, mannitol); incorporation of the material into particulate preparations of polymeric compounds such as polylactic acid, polyglycolic acid, etc. or into liposomes. Hylauronic acid may also be used. Such compositions may influence the physical state, stability, rate of *in vivo* release, and rate of *in vivo* clearance of the present proteins and derivatives. *See, e.g.*, Remington's Pharmaceutical Sciences, 18th Ed. [1990, Mack Publishing Co., Easton, PA 18042] pages 1435-1712 which are herein

incorporated by reference. The compositions may be prepared in liquid form, or may be in dried powder, such as lyophilized form.

Oral Delivery. Contemplated for use herein are oral solid dosage forms, which are described generally in Remington's Pharmaceutical Sciences, 18th Ed.1990 (Mack Publishing Co. Easton PA 18042) at Chapter 89, which is herein incorporated by reference. Solid dosage forms include tablets, capsules, pills, troches or lozenges, cachets or pellets. Also, liposomal or proteinoid encapsulation may be used to formulate the present compositions (as, for example, proteinoid microspheres reported in U.S. Patent No. 4,925,673). Liposomal encapsulation may be used and the liposomes may be derivatized with various polymers (*e.g.*, U.S. Patent No. 5,013,556). A description of possible solid dosage forms for the therapeutic is given by Marshall, K. In: *Modern Pharmaceutics* Edited by G.S. Banker and C.T. Rhodes Chapter 10, 1979, herein incorporated by reference. In general, the formulation will include an agent of the present invention (or chemically modified forms thereof) and inert ingredients which allow for protection against the stomach environment, and release of the biologically active material in the intestine.

Also specifically contemplated are oral dosage forms of the above derivatized component or components. The component or components may be chemically modified so that oral delivery of the derivative is efficacious. Generally, the chemical modification contemplated is the attachment of at least one moiety to the component molecule itself, where said moiety permits (a) inhibition of proteolysis; and (b) uptake into the blood stream from the stomach or intestine. Also desired is the increase in overall stability of the component or components and increase in circulation time in the body. An example of such a moiety is polyethylene glycol.

For the component (or derivative) the location of release may be the stomach, the small intestine (the duodenum, the jejunum, or the ileum), or the large intestine. One skilled in the art has available formulations which will not dissolve in the stomach, yet will release the material in the duodenum or elsewhere in the intestine. Preferably, the release will avoid the deleterious effects of the stomach environment, either by

protection of the protein (or derivative) or by release of the biologically active material beyond the stomach environment, such as in the intestine.

The therapeutic can be included in the formulation as fine multi-particulates in the form of granules or pellets of particle size about 1 mm. The formulation of the material for capsule administration could also be as a powder, lightly compressed plugs or even as tablets. The therapeutic could be prepared by compression.

One may dilute or increase the volume of the therapeutic with an inert material. These diluents could include carbohydrates, especially mannitol, a-lactose, anhydrous lactose, cellulose, sucrose, modified dextrans and starch. Certain inorganic salts may be also be used as fillers including calcium triphosphate, magnesium carbonate and sodium chloride. Some commercially available diluents are Fast-Flo, Emdex, STA-Rx 1500, Emcompress and Avicell.

Disintegrants may be included in the formulation of the therapeutic into a solid dosage form. Materials used as disintegrates include but are not limited to starch, including the commercial disintegrant based on starch, Explotab. Binders also may be used to hold the therapeutic agent together to form a hard tablet and include materials from natural products such as acacia, tragacanth, starch and gelatin.

An anti-frictional agent may be included in the formulation of the therapeutic to prevent sticking during the formulation process. Lubricants may be used as a layer between the therapeutic and the die wall. Glidants that might improve the flow properties of the drug during formulation and to aid rearrangement during compression also might be added. The glidants may include starch, talc, pyrogenic silica and hydrated silicoaluminate.

In addition, to aid dissolution of the therapeutic into the aqueous environment a surfactant might be added as a wetting agent. Additives which potentially enhance uptake of the protein (or derivative) are for instance the fatty acids oleic acid, linoleic acid and linolenic acid.

Nasal Delivery. Nasal delivery of an agent of the present invention (or derivative) is also contemplated. Nasal delivery allows the passage of a peptide, for example, to the blood stream directly after administering the therapeutic product to the nose, without the necessity for deposition of the product in the lung. Formulations for nasal delivery include those with dextran or cyclodextran.

Transdermal administration. Various and numerous methods are known in the art for transdermal administration of a drug, *e.g.*, via a transdermal patch. Transdermal patches are described in for example, U.S. Patent No. 5,407,713, issued April 18, 1995 to Rolando *et al.*; U.S. Patent No. 5,352,456, issued October 4, 1004 to Fallon *et al.*; U.S. Patent No. 5,332,213 issued August 9, 1994 to D'Angelo *et al.*; U.S. Patent No. 5,336,168, issued August 9, 1994 to Sibalis; U.S. Patent No. 5,290,561, issued March 1, 1994 to Farhadieh *et al.*; U.S. Patent No. 5,254,346, issued October 19, 1993 to Tucker *et al.*; U.S. Patent No. 5,164,189, issued November 17, 1992 to Berger *et al.*; U.S. Patent No. 5,163,899, issued November 17, 1992 to Sibalis; U.S. Patent Nos. 5,088,977 and 5,087,240, both issued February 18, 1992 to Sibalis; U.S. Patent No. 5,008,110, issued April 16, 1991 to Benecke *et al.*; and U.S. Patent No. 4,921,475, issued May 1, 1990 to Sibalis, the disclosure of each of which is incorporated herein by reference in its entirety.

It can be readily appreciated that a transdermal route of administration may be enhanced by use of a dermal penetration enhancer, *e.g.*, such as enhancers described in U.S. Patent No. 5,164,189 (*supra*), U.S. Patent No. 5,008,110 (*supra*), and U.S. Patent No. 4,879,119, issued November 7, 1989 to Aruga *et al.*, the disclosure of each of which is incorporated herein by reference in its entirety.

Pulmonary Delivery. Also contemplated herein is pulmonary delivery of the pharmaceutical compositions of the present invention. A pharmaceutical composition of the present invention is delivered to the lungs of a mammal while inhaling and traverses across the lung epithelial lining to the blood stream. Other reports of this include Adjei *et al.* [*Pharmaceutical Research*, **7**:565-569 (1990); Adjei et al., *International Journal of Pharmaceutics*, **63**:135-144 (1990) (leuprolide acetate); Braquet *et al.*, *Journal of Cardiovascular Pharmacology*, **13(suppl. 5):**143-146 (1989)

(endothelin-1); Hubbard *et al., Annals of Internal Medicine*, **Vol. III**, pp. 206-212 (1989) (α1-antitrypsin); Smith *et al., J. Clin. Invest.*, **84**:1145-1146 (1989) (α-1-proteinase); Oswein *et al.*, "Aerosolization of Proteins", *Proceedings of Symposium on Respiratory Drug Delivery II*, Keystone, Colorado, March, (1990) (recombinant human growth hormone); Debs et al., *J. Immunol.*, **140**:3482-3488 (1988) (interferon-γ and tumor necrosis factor alpha); Platz *et al.*, U.S. Patent No. 5,284,656 (granulocyte colony stimulating factor)]. A method and composition for pulmonary delivery of drugs for systemic effect is described in U.S. Patent No. 5,451,569, issued September 19, 1995 to Wong *et al.*

A subject in whom administration of an agent of the present invention is an effective therapeutic regiment for cancer, for example, is preferably a human, but can be any animal. Thus, as can be readily appreciated by one of ordinary skill in the art, the methods and pharmaceutical compositions of the present invention are particularly suited to administration to any animal, *e.g.*, for veterinary medical use, particularly for a mammal, and including, but by no means limited to, domestic animals, such as feline or canine subjects, farm animals, including bovine, equine, caprine, ovine, and porcine subjects, wild animals (whether in the wild or in a zoological garden), research animals, such as mice, rats, rabbits, goats, sheep, pigs, dogs, cats, avian species, such as chickens, turkeys, and songbirds.

The present invention may be better understood by reference to the following non-limiting Example, which is provided as exemplary of the invention. The following example is presented in order to more fully illustrate the preferred embodiments of the invention. It should in no way be construed, however, as limiting the broad scope of the invention.

EXAMPLE

STRUCTURE AND LIGAND OF A HISTONE ACETYLTRANSFERASE BROMODOMAIN

Introduction

The bromodomain is a protein motif comprising approximately 110 amino acids that is found in practically all nuclear histone acetyltransferases (HATs) [Jeanmougin *et al.*, Trends in Biochemical *Sciences*, **22**:151-153 (1997)]. However, despite the seemingly requisite occurrence of this motif in HATs, their role in these enzymes is unknown. Indeed, although this motif has also been identified in other chromatin proteins, heretofore not even one binding partner for a bromodomain had been identified.

Materials and Methods

Sample preparation: The bromodomain of P/CAF (residues 719-832 of SEQ ID NO:2) was subcloned into the pET14b expression vector (Novagen) and expressed in *Escherichia coli* BL21(DE3) cells. Uniformly ^{15}N- and $^{15}N/^{13}C$-labelled proteins were prepared by growing bacteria in a minimal medium containing $^{15}NH_4Cl$ with or without $^{13}C_6$-glucose. A uniformly $^{15}N/^{13}C$-labelled and fractionally deuterated protein sample was prepared by growing the cells in 75% ^2H_2O. The bromodomain was purified by affinity chromatography on a nickel-IDA column (Invitrogen) followed by the removal of poly-His tag by thrombin cleavage. The final purification of the protein was achieved by size-exclusion chromatography. The acetyl-lysine-containing peptides were prepared on a MilliGen 9050 peptide synthesizer (Perkin Elmer) using Fmoc/HBTU chemistry. Acetyl-lysine was incorporated using the reagent Fmoc-Ac-Lys with HBTU/DIPEA activation. NMR samples contained approximately 1 mM protein in 100mM phosphate buffer of pH 6.5 and 5mM perdeuterated DTT and 0.5mM EDTA in $H_2O/^2H_2O$ (9/1) or ^2H_2O.

NMR spectroscopy: All NMR spectra were acquired at 30°C on a Bruker DRX600 or DRX500 spectrometer. The backbone assignments of the ^1H, ^{13}C, and ^{15}N resonances were achieved using deuterium-decoupled triple-resonance experiments of HNCACB and HN(CO)CACB [Yamazaki *et al.*, *J. Am. Chem. Soc.* **116**:11655-11666 (1994)] recorded using the uniformly $^{15}N/^{13}C$-labeled and fractionally deuterated protein. The

side-chain atoms were assigned from 3D HCCH-TOCSY [Clore and Gronenborn, *Meth. Enzymol.* **239**:249-363 (1994)] and (H)C(CO)NH-TOCSY [Logan *et al.*, *J. Biolmol. NMR* **3**:225-231 (1993)] data collected on the uniformly $^{15}N/^{13}C$-labeled protein. Stereospecific assignments of methyl groups of the Val and Leu residues were obtained using a fractionally ^{13}C-labeled sample [Neri *et al.*, *Biochemistry* **28**:7510-7516 (1989)]. The NOE-derived distance restraints were obtained from ^{15}N- or ^{13}C-edited 3D NOESY spectra. ϕ-angle restraints were determined based on the $^{3}J_{HN,H\alpha}$ coupling constants measured in a 3D HNHA spectrum [Clore and Gronenborn, *Meth. Enzymol.* **239**:249-363 (1994)]. Slowly exchanging amide protons were identified from a series of 2D ^{15}N-HSQC spectra recorded after the H_2O buffer was changed to a $^{2}H_2O$ buffer. The intermolecular NOEs used in defining the structure of the bromodomain/Ac-histamine complex were detected in ^{13}C-edited (F_1), $^{13}C/^{15}N$-filtered (F_3) 3D NOESY spectrum [Clore and Gronenborn, *Meth. Enzymol.* **239**:249-363 (1994)]. All NMR spectra were processed with the NMRPipe/NMRDraw programs and analyzed using NMRView [Johnson and Blevins, *J. Biomol., NMR* **4**:603-614 (1994)].

Structure calculations: Structures of the bromodomain were calculated with a distance geometry/simulated annealing protocol using the X-PLOR program [Brunger, A. *X-PLOR Version 3.1*: *A system for X-Ray crystallography and NMR*, Yale University Press, New Haven, CT, (1993)]. A total of 1324 manually assigned NOE-derived distance restraints were obtained from the ^{15}N- and ^{13}C-edited NOE spectra. Further analysis of the NOE spectra was carried out by the iterative automated assignment procedure using ARIA [Nilges and O'Donoghue, *Prog. NMR Spectroscopy* **32**:107-139 (1998)], which integrates with X-PLOR for structure calculations. A total of 1519 unambiguous and 590 ambiguous distance restraints were identified from the NOE data by ARIA, many of which were checked and confirmed manually. The ARIA-assigned distance restraints were in agreement with the structures calculated using only the manually assigned NOE distance restraints, 28 hydrogen-bond distance restraints for 14 hydrogen bonds, and 54 ϕ-angle restraints. The final structure calculations employed a total of 3515 NMR experimental restraints obtained from the manual and the ARIA-assisted assignments, 2843 of which were unambiguously assigned NOE-derived distance restraints that comprise of 1077 intra-residue, 621

sequential, 550 medium-range, and 595 long-range NOEs. For the ensemble of the final 30 structures, no distance and torsional angle restraints were violated by more than 0.3Å and 5°, respectively. The total, distance violation, and dihedral violation energies were 178.7 ± 2.4 kcal mol^{-1}, 41.6 ± 0.9 kcal mol^{-1}, and 0.50 ± 0.06 kcal mol^{-1}, respectively. The Lennard-Jones potential which was not used during any refinement stage, was -526.2 ± 16.8 kcal mol^{-1} for the final structures. Ramachandran plot analysis of the final structures (residues 727-828) with Procheck-NMR [Laskowski *et al., J. Biolmol. NMR* **8**:477-486 (1996)] showed that 71.0 ± 0.6%, 23.8 ± 0.6%, 3.5 ± 0.2%, and 1.7 ± 0.2% of the non-Gly and non-Pro residues were in the most favorable, additionally allowed, generously allowed, and disallowed regions, respectively. The corresponding values for the residues in the four α-helices (residues 727-743, 770-776, 785-802, and 807-827) were 88.9 ± 0.4%, 11.0 ± 0.4%, 0.1 ± 0.1%, and 0.0 ± 0.0%, respectively. The structure of the bromodomain/acetyl-histamine complex was determined using the free form structure and additional 25 intermolecular and 5 intra-ligand NOE-derived distance restraints.

Site-directed mutagenesis: Mutant proteins were prepared using the QuickChange site-directed mutagenesis kit (Stratagene). The presence of appropriate mutations was confirmed by DNA sequencing.

Ligand titration: Ligand titration experiments were performed by recording a series of 2D ^{15}N- and ^{13}C-HSQC spectra on the uniformly ^{15}N-, and $^{15}N/^{13}C$-labelled bromodomain (~0.3mM), respectively, in the presence of different amounts of ligand concentration ranging from 0 to approximately 2.0 mM. The protein sample and the stock solutions of the ligands were all prepared in the same aqueous buffer containing 100mM phosphate and 5mM perdeuterated DTT at pH 6.5.

The full length nucleic acid sequence of the human p300/CBP-associated factor (P/CAF) was obtained from GenBank. Accession No: U57317.2 (SEQ ID NO:1) :

```
   1 ggggccgcgt cgacgcggaa aagaggccgt ggggggcctc ccagcgctgg cagacaccgt
  61 gaggctggca gccgccggca cgcacaccta gtccgcagtc ccgaggaaca tgtccgcagc
 121 cagggcgcgg agcagagtcc cgggcaggag aaccaaggga gggcgtgtgc tgtggcggcg
 181 gcggcagcgg cagcggagcc gctagtcccc tccctcctgg gggagcagct gccgccgctg
 241 ccgccgccgc caccaccatc agcgcgcggg gcccggccag agcgagccgg gcgagcggcg
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301 cgctaggggg agggcggggg cggggagggg ggtgggcgaa gggggcggga gggcgtgggg
361 ggagggtctc gctctcccga ctaccagagc ccgagggaga ccctggcggc ggcggcggcg
421 cctgacactc ggcgcctcct gccgtgctcc ggggcggcat gtccgaggct ggcggggccg
481 ggccgggcgg ctgcggggca ggagccgggg caggggccgg gcccggggcg ctgccccgc
541 agcctgcggc gcttccgccc gcgcccccgc agggctcccc ctgcgccgct gccgccgggg
601 gctcgggcgc ctgcggtccg gcgacggcag tggctgcagc gggcacggcc gaaggaccgg
661 gaggcggtgg ctcggcccga atcgccgtga agaaagcgca actacgctcc gctccgcggg
721 ccaagaaact ggagaaactc ggagtgtact ccgcctgcaa ggccgaggag tcttgtaaat
781 gtaatggctg gaaaaaccct aacccctcac ccactccccc cagagccgac ctgcagcaaa
841 taattgtcag tctaacagaa tcctgtcgga gttgtagcca tgccctagct gctcatgttt
901 cccacctgga gaatgtgtca gaggaagaaa tgaacagact cctgggaata gtattggatg
961 tggaatatct ctttacctgt gtccacaagg aagaagatgc agataccaaa caagtttatt
1021 tctatctatt taagctcttg agaaagtcta ttttacaaag aggaaaacct gtggttgaag
1081 gctctttgga aaagaaaccc ccatttgaaa aacctagcat tgaacagggt gtgaataact
1141 ttgtgcagta caaatttagt cacctgccag caaaagaaag gcaaacaata gttgagttgg
1201 caaaaatgtt cctaaaccgc atcaactatt ggcatctgga ggcaccatct caacgaagac
1261 tgcgatctcc caatgatgat atttctggat acaaagagaa ctacacaagg tggctgtgtt
1321 actgcaacgt gccacagttc tgcgacagtc tacctcggta cgaaaccaca caggtgtttg
1381 ggagaacatt gcttcgctcg gtcttcactg ttatgaggcg acaactcctg gaacaagcaa
1441 gacaggaaaa agataaactg cctcttgaaa aacgaactct aatcctcact catttcccaa
1501 aatttctgtc catgctagaa gaagaagtat atagtcaaaa ctctcccatc tgggatcagg
1561 attttctctc agcctcttcc agaaccagcc agctaggcat ccaaacagtt atcaatccac
1621 ctcctgtggc tgggacaatt tcatacaatt caacctcatc ttcccttgag cagccaaacg
1681 cagggagcag cagtcctgcc tgcaaagcct cttctggact tgaggcaaac ccaggagaaa
1741 agaggaaaat gactgattct catgttctgg aggaggccaa gaaaccccga gttatggggg
1801 atattccgat ggaattaatc aacgaggtta tgtctaccat cacggaccct gcagcaatgc
1861 ttggaccaga gaccaatttt ctgtcagcac actcggccag ggatgaggcg gcaaggttgg
1921 aagagcgcag gggtgtaatt gaatttcacg tggttggcaa ttcccctcaac cagaaaccaa
1981 acaagaagat cctgatgtgg ctggttggcc tacagaacgt tttctcccac cagctgcccc
2041 gaatgccaaa agaatacatc acacggctcg tctttgaccc gaaacacaaa acccttgctt
2101 taattaaaga tggccgtgtt attggtggta tctgtttccg tatgttccca tctcaaggat
2161 tcacagagat tgtcttctgt gctgtaacct caaatgagca agtcaagggc tatggaacac
2221 acctgatgaa tcatttgaaa gaatatcaca taaagcatga catcctgaac ttcctcacat
2281 atgcagatga atatgcaatt ggatacttta agaaacaggg tttctccaaa gaaattaaaa
2341 tacctaaaac caaatatgtt ggctatatca aggattatga aggagccact ttaatgggat
2401 gtgagctaaa tccacggatc ccgtacacag aattttctgt catcattaaa aagcagaagg
2461 agataattaa aaaactgatt gaaagaaaac aggcacaaat tcgaaaagtt taccctggac
2521 tttcatgttt taaagatgga gttcgacaga ttcctataga aagcattcct ggaattagag
2581 agacaggctg gaaaccgagt ggaaaagaga aaagtaaaga gcccagagac cctgaccagc
2641 tttacagcac gctcaagagc atcctccagc aggtgaagag ccatcaaagc gcttggccct
2701 tcatggaacc tgtgaagaga acagaagctc caggatatta tgaagttata aggttcccca
2761 tggatctgaa aaccatgagt gaacgcctca agaataggta ctacgtgtct aagaaattat
2821 tcatggcaga cttacagcga gtctttacca attgcaaaga gtacaacgcc gctgagagtg
2881 aatactacaa atgtgccaat atcctggaga aattcttctt cagtaaaatt aaggaagctg
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2941 gattaattga caagtgattt tttttccccc tctgcttctt agaaactcac caagcagtgt
3001 gcctaaagca aggt
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The full length protein sequence of the human p300/CBP-associated factor (P/CAF) was obtained from GenBank. Accession No: U57317.2, (SEQ ID NO:2):

```
1   MSEAGGAGPG GCGAGAGAGA GPGALPPQPA ALPPAPPQGS PCAAAAGGSG ACGPATAVAA
61  AGTAEGPGGG GSARIAVKKA QLRSAPRAKK LEKLGVYSAC KAEESCKCNG WKNPNPSPTP
121 PRADLQQIIV SLTESCRSCS HALAAHVSHL ENVSEEEMNR LLGIVLDVEY LFTCVHKEED
181 ADTKQVYFYL FKLLRKSILQ RGKPVVEGSL EKKPPFEKPS IEQGVNNFVQ YKFSHLPAKE
241 RQTIVELAKM FLNRINYWHL EAPSQRRLRS PNDDISGYKE NYTRWLCYCN VPQFCDSLPR
301 YETTQVFGRT LLRSVFTVMR RQLLEQARQE KDKLPLEKRT LILTHFPKFL SMLEEEVYSQ
361 NSPIWDQDFL SASSRTSQLG IQTVINPPPV AGTISYNSTS SSLEQPNAGS SSPACKASSG
421 LEANPGEKRK MTDSHVLEEA KKPRVMGDIP MELINEVMST ITDPAAMLGP ETNFLSAHSA
481 RDEAARLEER RGVIEFHVVG NSLNQKPNKK ILMWLVGLQN VFSHQLPRMP KEYITRLVFD
541 PKHKTLALIK DGRVIGGICF RMFPSQGFTE IVFCAVTSNE QVKGYGTHLM NHLKEYHIKH
601 DILNFLTYAD EYAIGYFKKQ GFSKEIKIPK TKYVGYIKDY EGATLMGCEL NPRIPYTEFS
661 VIIKKQKEII KKLIERKQAQ IRKVYPGLSC FKDGVRQIPI ESIPGIRETG WKPSGKEKSK
721 EPRDPDQLYS TLKSILQQVK SHQSAWPFME PVKRTEAPGY YEVIRFPMDL KTMSERLKNR
781 YYVSKKLFMA DLQRVFTNCK EYNAAESEYY KCANILEKFF FSKIKEAGLI DK
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Results

The P/CAF bromodomain represents an extensive family of bromodomains (Figure 1). A large number of long-range nuclear Overhauser enhancement (NOE)-derived distance restraints were identified in the NMR data of the P/CAF bromodomain, yielding a well-defined three-dimensional structure (Figures 2A -2D). Table 1 shows the NMR chemical shift assignment of the P/CAF bromodomain. Table 2 shows the Unambiguous NOE-derived distance restraints. Table 3 shows the Ambiguous NOE-derived distance restraints. Table 4 shows the Hydrogen bond restraints. The NMR structure coordinates of the P/CAF bromodomain in the free and complexed to acetyl-histamine are shown in Tables 5 and 6, respectively.

The structure consists of a four-helix bundle (helices α_Z, α_A, α_B, and α_C) with a left-handed twist, and a long intervening loop between helices α_Z and α_A (termed the ZA loop, Figure 2E). The four amphipathic α-helices are packed tightly against one another in an antiparallel manner, with crossing angles for adjacent helices of ~16-20°. The up-and-down four-helix bundle can adapt two topological folds with opposite

handedness (Figures 2F-2G). The right-handed four-helix bundle fold occurs more commonly and is seen in proteins such as hemerythrin and cytochrome b_{562}. The left-handed fold of the bromodomain structure is less common, but also observed in proteins such as cytochrome b_5 and T4 lysozyme [Richardson, J., *Adv.Protein Chem.*, **34**:167-339 (1989); Presnell and Cohen, *Proc. Natl. Acad. Sci. USA* **86**:6592-6596 (1989)]. This topological difference arises from the orientation of the loop between the first two helices (Fig. 2F-2G). The right-handed four-helix bundle proteins have a relatively short hairpin-like connection between the first two helices, which makes the "preferred" turn to the right at the top of the first helix [Richardson, J., *Adv.Protein Chem.*, **34**:167-339 (1989); Presnell and Cohen, *Proc. Natl. Acad. Sci. USA* **86**:6592-6596 (1989); Weber and Salemme, *Nature* **287**:82-84 (1980)]. In contrast, proteins with the left-handed fold usually have a long loop after the first helix and often contain additional secondary structural elements at the base of the helix bundle [Richardson, J., *Adv.Protein Chem.*, **34**:167-339 (1989); Presnell and Cohen, *Proc. Natl. Acad. Sci. USA* **86**:6592-6596 (1989)]. In the bromodomain structure, this long ZA loop has a defined conformation and is packed against the loop between helices α_B and α_C (termed the BC loop) to form a hydrophobic pocket. These tertiary interactions between the two loops appear to favor the left turn of the ZA loop, resulting in the left-handed four-helix bundle fold of the bromodomain. The hydrophobic pocket formed by loops ZA and BC is lined by residues Val752, Ala757, Tyr760, Val763, Tyr802 and Tyr809 (Fig. 2H), and appears to be a site for protein-protein interactions (see below). The pocket is located at one end of the four-helix bundle, opposite to the N- and C-termini of the protein. Interestingly, the ZA loop varies in length amongst different bromodomains, but almost always contains residues corresponding to Phe748, Pro751, Pro758, Tyr760, and Pro767 (Figure 1). The conservation of these residues within the ZA loop as well as residues within the α-helical regions implies a similar left-handed four-helix bundle structure for the large family of bromodomains (Fig. 1).

The modular bromodomain structure supports the idea that bromodomain can act as a functional unit for protein-protein interactions. The observation that bromodomains are found in nearly all known nuclear HATs (A-type) that are known to promote transcription-related acetylation of histones on specific lysine residues, but not present in cytoplasmic HATs (B-type), prompted the determination of whether bromodomains

can interact with acetyl-lysine (AcK). The NMR titration of the P/CAF bromodomain were performed with a peptide (SGRGKGG-AcK-GLGK) derived from histone H4, in which Lys8 is acetylated (Lys8 is the major acetylation site in H4 for GCN5, a yeast homologue of P/CAF). Remarkably, the bromodomain could indeed bind the AcK peptide. Moreover, this interaction appeared to be specific, based on the ^{15}N-HSQC spectra which showed that only a limited number of residues underwent chemical shift changes as a function of peptide concentration (Figure 3A). Conversely, the NMR titration of the bromodomain with a non-acetylated, but otherwise identical H4 peptide, showed no noticeable chemical shift changes, demonstrating that the interaction between the bromodomain and the lysine-acetylated H4 peptide was dependent upon acetylation of lysine. The dissociation constant (K_D) for the AcK peptide was estimated to be 346 ± 54 μM. This binding is likely reinforced through additional interactions between bromodomain-containing proteins and target proteins. Notably, many chromatin-associated proteins contain two or multiple bromodomains (Figure 1). Indeed, binding with another lysine-acetylated peptide (RKSTGG-AcK-APRKQ) derived from the major acetylation site on histone H3 (residues 9-20) was also observed. Together, these data demonstrate that the P/CAF bromodomain has the ability to bind AcK peptides in an acetylation dependent manner.

Intriguingly, the bromodomain residues that exhibited the most significant ^{1}H and ^{15}N chemical shift changes on peptide binding are located near the hydrophobic pocket between the ZA and BC loops (Figure 3B). Because a similar pattern of amide chemical shift changes was observed with the two different AcK-containing peptides, it was surmised that the hydrophobic cavity is the primary binding site for AcK. This hypothesis was further supported by titration with acetyl-histamine, which mimics the chemical structure of the AcK side-chain (Figure 3C). Both ^{15}N- and ^{13}C-HSQC spectra showed that interaction with acetyl-histamine was also acetylation-dependent, involving the same set of residues that showed chemical shift perturbations with similar concentration dependence. It should be noted that the bromodomain did not bind to the amino acids acetyl-lysine or acetyl-histidine alone, possibly due to the presence of the charged amino, carboxyl, or caboxylate group adjacent to the acetyl moiety (Figure 3C). Taken together, these results strongly suggest that the P/CAF

bromodomain can interact with acetyl-lysine-containing proteins in a specific manner, and that this interaction is localized to the bromodomain hydrophobic cavity.

To identify the key residues involved in bromodomain-AcK recognition, the NMR structure of the P/CAF bromodomain in complex with acetyl-histamine was elucidated. As anticipated, the acetylated moiety binds in the bromodomain hydrophobic pocket (Figure 4). The intermolecular interactions are largely hydrophobic in nature, with the methyl group of acetyl-histamine making extensive contacts with the side-chains of Val752, Ala757, and Tyr760, and the methylene groups of acetyl-histamine displaying specific NOEs to Val752, Ala757, Tyr760, Tyr802, and Tyr809. No intermolecular NOEs were observed for the imidazole ring of acetyl-histamine. From the spectral analysis it is clear that the structure of the bromodomain is very similar in both the free and complex forms.

It is worth noting that the bromodomain-AcK recognition is reminiscent of the interactions between the histone acetyltransferase Hat1 and acetyl-CoA. Although the binding pockets of these two otherwise structurally unrelated proteins are composed of different secondary structural elements, the nature of acetyl-lysine recognition has striking similarities. In particular, Tyr809, Tyr802, Tyr760, and Val752 in the bromodomain appear to be related to Phe220, Phe261, Val254, and Ile217 of Hat1, respectively, in their interactions with the acetyl moiety. This observation may suggest an evolutionary convergent mechanism of acetyl-lysine recognition between bromodomains and histone acetyltransferases.

To determine the relative contributions of residues within the hydrophobic cavity in bromodomain-AcK binding, site-directed mutagenesis was used to alter residues Tyr809, Tyr802, Tyr760, and Val752 (Table 7).

Table 7. Structural and Functional Analysis of the P/CAF Bromodomain Mutants

Bromodomain Proteins	Structural Integrity [a]	H4 AcK-Peptide Binding K_D (μM) [b]
Wild-Type	++++	346 ± 54
Tyr809Ala	++++	No Binding [c]
Tyr802Ala	+++	> 10,000 [d]
Tyr760Ala	+++	> 10,000
Val752Ala	++	> 10,000

a. The effects of mutations on the structural integrity of the bromodomain were assessed by using the ^{15}N-HSQC spectra. The amide ^{1}H/^{15}N resonances of the mutant proteins were compared to those of the wild-type bromodomain to determine if the particular mutations lead to global or local structure disruption. Severe line-broadening of the amide resonances would indicate protein conformational exchange due to a decrease of structure stability resulting from point mutations. Structural integrity of the mutant proteins is expressed here relative to that of the wild-type, using the signs of "++++" for as stable as the wild-type, "+++" for mildly destabilized, "++" for moderately destabilized, and "–" for completely unfolded.

b. The ligand binding affinity (K_D) of the bromodomain proteins was estimated by following chemical shift changes of amide peaks in the ^{15}N-HSQC spectra as a function of the ligand concentration.

c. No detectable ligand binding observed in the NMR titration.

d. Ligand binding affinity was significantly reduced and beyond the limit for reliable measurements by NMR titration.

Substitution of Ala for Tyr809 completely abrogated the bromodomain binding to the lysine-acetylated H4 peptide, while the Tyr802Ala, Tyr760Ala, and Val752Ala mutants had significantly reduced ligand binding affinity. To assess whether these mutations disrupted the overall bromodomain fold, the ^{15}N-HSQC spectra of the mutants was compared to that of the wild-type protein. For the Tyr809Ala mutant, the amide chemical shifts were only affected for a few residues near the mutation site. However, mutations of the other residues in the hydrophobic binding pocket perturbed the local protein conformation to greater extents, particularly the ZA loop (Table 7). Thus, the NMR structural analysis and the mutagenesis studies show that Tyr809, which is structurally supported by Trp746 and Asn803 (Fiure 4), is essential for the bromodomain interaction with the acetyl group of acetyl-lysine, while residues of Tyr802, Tyr760, and Val752 likely play both structural and functional roles in the recognition. These residues are highly conserved throughout the bromodomain family (Figure 1), suggesting that recognition of acetyl-lysine may be a feature of bromodomains, in general. Therefore, Val752, Ala757, Tyr760, Tyr802, Asn803, and Tyr809 are key amino acid residues for the P/CAF bromodomain binding to acetyl-lysine.

Table 8:Amino Acid Sequences of Bromodomains Identified in Figure 1

PROTEIN **BD**	SEQ ID NO:	GenBank Acc. No.	PROTEIN **BD**	SEQ ID NO:	GenBank Acc. No.
hsp/CAF	7	U57317	dmFSH-2	25	
hsGCN5	8	U57136	scBDF1-2	26	
ttP55	9	U47321	hsBR140	27	JC2069
scGCN5	10	Q03330	hsSMAP	28	X87613
hsP300	11	A54277	ggPB1-1	29	X90849
hsCBP	12	S39162	ggPB1-2	30	
mmCBP	13	S39161	ggPB1-3	31	
ceYNJ1	14	P34545	ggPB1-4	32	
hsCCG1-1	15	P21675	ggPB1-5	33	
msCCG1-1	16	D26114	spBRO-1	34	S54260
hsCCG1-2	17		spBRO-2	35	
msCCG1-2	18		hsSNF2a	36	S45251
hsRing3-1	19	P25440	hsBRG1	37	S39039
hsORFX-1	20	D26362	ggBRM	38	X91638
dmFSH-1	21	P13709	ggBRG1	39	X91637
scBDF1-1	22	P35817	hsTIF1b	40	X97548
hsRing3-2	23		mmTIF1b	41	X99644
hsORFX-2	24		mmTIF1a	42	S78219

The present invention is not to be limited in scope by the specific embodiments described herein. Indeed, various modifications of the invention in addition to those described herein will become apparent to those skilled in the art from the foregoing description and the accompanying figures. Such modifications are intended to fall within the scope of the appended claims.

It is further to be understood that all base sizes or amino acid sizes, and all molecular weight or molecular mass values, given for nucleic acids or polypeptides are approximate, and are provided for description.

Various publications are cited herein, the disclosures of which are hereby incorporated by reference herein in their entireties.

Table 1

NMR Chemical Shift Assignment of the P/CAF Bromodomain

```
RES_ID          715
RES_TYPE        GLY
SPIN_SYSTEM_ID  1
HETEROGENEITY   100
END_RES_DEF

RES_ID          716
RES_TYPE        SER
SPIN_SYSTEM_ID  2
HETEROGENEITY   100
END_RES_DEF

RES_ID          717
RES_TYPE        HIS
SPIN_SYSTEM_ID  3
HETEROGENEITY   100
END_RES_DEF

RES_ID          718
RES_TYPE        MET
SPIN_SYSTEM_ID  4
HETEROGENEITY   100
END_RES_DEF

RES_ID          719
RES_TYPE        SER
SPIN_SYSTEM_ID  5
HETEROGENEITY   100
END_RES_DEF

RES_ID          720
RES_TYPE        LYS
SPIN_SYSTEM_ID  6
HETEROGENEITY   100
  CA  56.296000
  HA  4.361000
  CB  33.140000
  HB1  1.882000
  HB2  1.684000
  CG  25.430000
  HG1  1.585000
  HG2  1.433000
  CD  29.834000
  HD1  1.703000
  CE  41.960000
  HE1  3.003000
END_RES_DEF

RES_ID          721
RES_TYPE        GLU
SPIN_SYSTEM_ID  7
HETEROGENEITY   100
  N  122.990000
  HN  8.317000
  CA  54.620000
  HA  4.540000
  CB  29.830000
  HB1  2.024000
  HB2  1.893000
  CG  35.893000
  HG1  2.271000
END_RES_DEF

RES_ID          722
RES_TYPE        PRO
SPIN_SYSTEM_ID  8
HETEROGENEITY   100
  CA  63.430000
  HA  4.393000
  CB  32.030000
  HB1  2.224000
  HB2  1.880000
  CG  27.630000
  HG1  2.028000
  CD  50.760000
  HD2  3.656000
  HD1  3.800000
END_RES_DEF

RES_ID          723
RES_TYPE        ARG
SPIN_SYSTEM_ID  9
HETEROGENEITY   100
  N  121.192000
  HN  8.416000
  CA  63.430000
  HA  4.331000
  CB  30.930000
  HB1  1.815000
  HB2  1.762000
  CG  27.630000
  HG1  1.681000
  CD  43.603000
  HD1  3.161000
END_RES_DEF

RES_ID          724
RES_TYPE        ASP
SPIN_SYSTEM_ID  10
HETEROGENEITY   100
  N  122.012000
  HN  8.273000
  CA  52.415000
  HA  4.874000
  CB  41.400000
  HB1  2.754000
  HB2  2.692000
END_RES_DEF

RES_ID          725
RES_TYPE        PRO
SPIN_SYSTEM_ID  11
HETEROGENEITY   100
  CA  65.080000
  HA  4.329000
  CB  32.590000
  HB1  2.326000
  HB2  1.973000
  CG  27.632000
  HG1  2.028000
  CD  51.310000
  HD1  3.866000
END_RES_DEF

RES_ID          726
RES_TYPE        ASP
SPIN_SYSTEM_ID  12
HETEROGENEITY   100
  N  119.716000
  HN  8.397000
  CA  55.720000
  HA  4.692000
  CB  40.550000
  HB1  2.792000
  HB2  2.730000
END_RES_DEF

RES_ID          727
RES_TYPE        GLN
SPIN_SYSTEM_ID  13
HETEROGENEITY   100
  N  121.356000
  HN  8.196000
  CA  55.920000
  HA  4.163000
  CB  28.730000
  HB1  2.148000
  CG  34.240000
  HG1  2.524000
  HG2  2.371000
END_RES_DEF

RES_ID          728
RES_TYPE        LEU
SPIN_SYSTEM_ID  14
HETEROGENEITY   100
  N  121.356000
  HN  8.210000
  CA  58.473000
  HA  4.045000
  CB  41.400000
  HB1  1.847000
  HB2  1.555000
  CG  27.080000
  HG  1.480000
  CD1  25.970000
  HD1#  0.794000
  CD2  23.226000
  HD2#  0.786000
END_RES_DEF

RES_ID          729
RES_TYPE        TYR
SPIN_SYSTEM_ID  15
HETEROGENEITY   100
  N  119.060000
  HN  8.021000
  CA  62.320000
  HA  4.038000
  CB  38.640000
  HB1  3.211000
  HB2  3.024000
  CD1  134.350000
  HD1  7.053000
  CE1  119.481000
  HE1  6.882000
END_RES_DEF

RES_ID          730
RES_TYPE        SER
SPIN_SYSTEM_ID  16
HETEROGENEITY   100
  N  112.173000
  HN  8.167000
  HA  3.920000
  HB1  3.995000
END_RES_DEF

RES_ID          731
RES_TYPE        THR
SPIN_SYSTEM_ID  17
HETEROGENEITY   100
  N  120.372000
  HN  8.059000
  CA  66.730000
  HA  3.924000
  CB  68.910000
  HB  4.247000
  CG2  21.570000
  HG2#  1.142000
END_RES_DEF

RES_ID          732
RES_TYPE        LEU
SPIN_SYSTEM_ID  18
HETEROGENEITY   100
  N  120.536000
  HN  8.460000
  CA  57.920000
  HA  3.289000
  CB  39.750000
  HB1  1.532000
  HB2  0.294000
  CG  24.880000
  HG  1.683000
  CD1  25.429000
  HD1#  0.469000
  CD2  19.921000
  HD2#  -0.193000
END_RES_DEF

RES_ID          733
RES_TYPE        LYS
SPIN_SYSTEM_ID  19
HETEROGENEITY   100
  N  118.568000
  HN  8.563000
  CA  60.125000
  HA  3.679000
  CB  32.588000
  HB1  1.729000
  HB2  1.360000
  CG  24.880000
  HG1  1.280000
  CD  29.835000
  HD1  1.585000
  CE  41.960000
  HE1  2.918000
END_RES_DEF

RES_ID          734
RES_TYPE        SER
SPIN_SYSTEM_ID  20
HETEROGENEITY   100
  N  113.157000
  HN  7.540000
  CA  61.227000
  HA  4.281000
  CB  63.879000
  HB1  4.060000
END_RES_DEF

RES_ID          735
RES_TYPE        ILE
SPIN_SYSTEM_ID  21
HETEROGENEITY   100
  N  120.700000
  HN  7.951000
  CA  65.080000
  HA  3.786000
  CB  38.095000
  HB  1.879000
  CG1  28.733000
  HG11  1.748000
  HG12  1.052000
  CG2  17.168000
  HG2#  1.003000
  CD1  13.863000
  HD1#  0.619000
END_RES_DEF

RES_ID          736
RES_TYPE        LEU
SPIN_SYSTEM_ID  22
HETEROGENEITY   100
  N  119.880000
  HN  8.841000
  CA  58.473000
  HA  4.090000
  CB  41.950000
  HB1  2.090000
  HB2  1.703000
  CG  27.330000
  HG  1.759000
  CD1  26.530000
  HD1#  1.061000
  CD2  23.776000
  HD2#  0.977000
END_RES_DEF

RES_ID          737
RES_TYPE        GLN
SPIN_SYSTEM_ID  23
HETEROGENEITY   100
  N  117.256000
  HN  8.505000
  CA  59.020000
  HA  4.032000
  CB  28.182000
  HB1  2.327000
  HB2  2.263000
  CG  34.240000
  HG1  2.536000
  HG2  2.461000
END_RES_DEF

RES_ID          738
RES_TYPE        GLN
SPIN_SYSTEM_ID  24
HETEROGENEITY   100
  N  118.896000
  HN  8.033000
  CA  59.574000
  HA  4.196000
  CB  29.835000
  HB1  2.482000
  HB2  2.469000
  CG  35.342000
  HG1  2.840000
  HG2  2.467000
  NE2  110.369000
  HE21  7.022000
  HE22  6.916000
END_RES_DEF

RES_ID          739
RES_TYPE        VAL
SPIN_SYSTEM_ID  25
HETEROGENEITY   100
  N  119.716000
  HN  8.526000
  CA  67.830000
  HA  3.844000
  CB  32.030000
  HB  2.384000
  CG1  23.330000
  HG1#  1.183000
  CG2  22.120000
  HG2#  1.033000
END_RES_DEF

RES_ID          740
RES_TYPE        LYS
SPIN_SYSTEM_ID  26
HETEROGENEITY   100
  N  114.633000
  HN  8.572000
  CA  59.574000
  HA  3.886000
  CB  32.380000
  HB1  1.873000
  HG1  1.022000
  HD1  1.520000
END_RES_DEF

RES_ID          741
RES_TYPE        SER
```

```
  SPIN_SYSTEM_ID  27
  HETEROGENEITY   100
    N  110.369000
    HN  7.557000
    CA  59.024000
    HA  4.448000
    CB  63.980000
    HB1  4.004000
  END_RES_DEF

  RES_ID          742
  RES_TYPE        HIS
  SPIN_SYSTEM_ID  28
  HETEROGENEITY   100
    N  125.619000
    HN  7.536000
    CA  58.473000
    HA  3.967000
    CB  32.588000
    HB1  2.990000
    HB2  2.799000
    CD2  118.930000
    HD2  4.978000
    CE1  138.755000
    HE1  7.522000
  END_RES_DEF

  RES_ID          743
  RES_TYPE        GLN
  SPIN_SYSTEM_ID  29
  HETEROGENEITY   100
    N  128.571000
    HN  8.543000
    CA  59.125000
    HA  4.209000
    CB  29.834000
    HB1  2.111000
    CG  33.690000
    HG1  2.390000
    NE2  112.173000
    HE21  7.581000
    HE22  6.870000
  END_RES_DEF

  RES_ID          744
  RES_TYPE        SER
  SPIN_SYSTEM_ID  30
  HETEROGENEITY   100
    N  119.060000
    HN  11.668000
    CA  60.125000
    HA  4.838000
    CB  63.980000
    HB1  4.334000
    HB2  3.926000
  END_RES_DEF

  RES_ID          745
  RES_TYPE        ALA
  SPIN_SYSTEM_ID  31
  HETEROGENEITY   100
    N  117.584000
    HN  7.868000
    CA  53.510000
    HA  4.396000
    CB  20.470000
    HB#  1.688000
  END_RES_DEF

  RES_ID          746
  RES_TYPE        TRP
  SPIN_SYSTEM_ID  32
  HETEROGENEITY   100
    N  116.600000
    HN  7.135000
    CA  60.691000
    HA  4.368000
    CB  27.630000
    HB1  3.594000
    HB2  3.351000
    CD1  128.843000
    HD1  7.897000
    NE1  110.861000
    HE1  10.474000
    CE3  122.234000
    HE3  7.336000
    CZ2  116.177000
    HZ2  7.382000
    CZ3  123.336000
    HZ3  7.197000
    CH2  126.089000
    HH2  7.150000
  END_RES_DEF

  RES_ID          747
  RES_TYPE        PRO
  SPIN_SYSTEM_ID  33
  HETEROGENEITY   100
    CA  64.531000
    HA  3.756000
    CB  29.835000
    HB1  0.487000
    HB2  -0.783000
    CG  26.530000
    HG1  0.233000
    HG2  -0.931000
    CD  50.212000
    HD2  1.567000
    HD1  2.177000
  END_RES_DEF

  RES_ID          748
  RES_TYPE        PHE
  SPIN_SYSTEM_ID  34
  HETEROGENEITY   100
    N  113.321000
    HN  7.585000
    CA  55.719000
    HA  4.930000
    CB  39.202000
    HB1  3.491000
    HB2  2.532000
    CD1  133.248000
    HD1  7.099000
    HE1  7.174000
    HZ  7.296000
  END_RES_DEF

  RES_ID          749
  RES_TYPE        MET
  SPIN_SYSTEM_ID  35
  HETEROGENEITY   100
    N  117.748000
    HN  7.115000
    CA  56.820000
    HA  4.286000
    CB  32.590000
    HB1  2.233000
    HB2  2.174000
    CG  33.140000
    HG1  2.851000
    CE  17.168000
    HE#  2.175000
  END_RES_DEF

  RES_ID          750
  RES_TYPE        GLU
  SPIN_SYSTEM_ID  36
  HETEROGENEITY   100
    N  113.813000
    HN  7.709000
    CA  53.516000
    HA  4.849000
    CB  31.487000
    HB1  2.091000
    HB2  1.730000
    CG  35.893000
    HG1  2.164000
  END_RES_DEF

  RES_ID          751
  RES_TYPE        PRO
  SPIN_SYSTEM_ID  37
  HETEROGENEITY   100
    CA  62.879000
    HA  4.242000
    CB  32.040000
    HB1  2.328000
    HB2  1.683000
    CG  27.080000
    HG1  2.126000
    HG2  1.978000
    CD  50.763000
    HD1  3.670000
  END_RES_DEF

  RES_ID          752
  RES_TYPE        VAL
  SPIN_SYSTEM_ID  38
  HETEROGENEITY   100
    N  124.450000
    HN  8.124000
    CA  63.430000
    HA  3.553000
    CB  32.580000
    HB  1.145000
    CG1  21.573000
    HG1#  0.464000
    CG2  21.573000
    HG2#  0.169000
  END_RES_DEF

  RES_ID          753
  RES_TYPE        LYS
  SPIN_SYSTEM_ID  39
  HETEROGENEITY   100
    N  129.883000
    HN  9.045000
    CA  56.310000
    HA  4.370000
    CB  32.880000
    HB1  1.873000
    HG1  1.435000
    HD1  1.673000
    HE1  2.985000
  END_RES_DEF

  RES_ID          754
  RES_TYPE        ARG
  SPIN_SYSTEM_ID  40
  HETEROGENEITY   100
    N  120.208000
    HN  8.054000
  END_RES_DEF

  RES_ID          755
  RES_TYPE        THR
  SPIN_SYSTEM_ID  41
  HETEROGENEITY   100
    CA  63.430000
    HA  4.038000
    CB  68.380000
    HB  4.293000
    CG2  22.670000
    HG2#  1.267000
  END_RES_DEF

  RES_ID          756
  RES_TYPE        GLU
  SPIN_SYSTEM_ID  42
  HETEROGENEITY   100
    N  118.732000
    HN  7.209000
    CA  56.270000
    HA  4.448000
    CB  30.930000
    HB1  2.174000
    HB2  2.000000
    CG  36.440000
    HG1  2.292000
  END_RES_DEF

  RES_ID          757
  RES_TYPE        ALA
  SPIN_SYSTEM_ID  43
  HETEROGENEITY   100
    N  122.504000
    HN  7.379000
    CA  50.220000
    HA  4.937000
    CB  19.370000
    HB#  1.082000
  END_RES_DEF

  RES_ID          758
  RES_TYPE        PRO
  SPIN_SYSTEM_ID  44
  HETEROGENEITY   100
    CA  65.080000
    HA  4.496000
    CB  31.487000
    HB1  2.374000
    HB2  2.027000
    CG  27.632000
    HG1  2.122000
    HG2  2.038000
    CD  50.212000
    HD2  3.515000
    HD1  3.717000
  END_RES_DEF

  RES_ID          759
  RES_TYPE        GLY
  SPIN_SYSTEM_ID  45
  HETEROGENEITY   100
  END_RES_DEF

  RES_ID          760
  RES_TYPE        TYR
  SPIN_SYSTEM_ID  46
  HETEROGENEITY   100
    N  122.504000
    HN  7.945000
    CA  62.328000
    HA  3.536000
    CB  39.750000
    HB1  2.689000
    HB2  2.487000
    CD1  133.799000
    HD1  5.120000
    CE1  118.379000
    HE1  6.070000
  END_RES_DEF

  RES_ID          761
  RES_TYPE        TYR
  SPIN_SYSTEM_ID  47
  HETEROGENEITY   100
    N  113.157000
    HN  8.225000
    CA  60.676000
    HA  4.101000
    CB  37.550000
    HB1  3.189000
    HB2  2.801000
    CD1  134.901000
    HD1  7.342000
    CE1  118.930000
    HE1  6.646000
  END_RES_DEF

  RES_ID          762
  RES_TYPE        GLU
  SPIN_SYSTEM_ID  48
  HETEROGENEITY   100
    N  117.912000
    HN  7.702000
    CA  57.922000
    HA  4.209000
    CB  29.480000
    HB1  2.086000
    CG  37.545000
    HG1  2.325000
    HG2  2.265000
  END_RES_DEF

  RES_ID          763
  RES_TYPE        VAL
  SPIN_SYSTEM_ID  49
  HETEROGENEITY   100
    N  115.453000
    HN  7.135000
    CA  63.430000
    HA  4.077000
    CB  33.690000
    HB  2.015000
    CG1  21.020000
    HG1#  1.045000
    CG2  21.574000
    HG2#  0.991000
  END_RES_DEF

  RES_ID          764
  RES_TYPE        ILE
  SPIN_SYSTEM_ID  50
  HETEROGENEITY   100
    N  122.832000
    HN  7.947000
    CA  57.920000
    HA  3.916000
    CB  34.240000
    HB  1.205000
    CG1  24.878000
    HG11  0.798000
    HG12  0.216000
    CG2  16.617000
    HG2#  0.380000
    CD1  9.457000
    HD1#  0.537000
  END_RES_DEF

  RES_ID          765
  RES_TYPE        ARG
  SPIN_SYSTEM_ID  51
  HETEROGENEITY   100
    N  125.291000
    HN  7.749000
    CA  57.371000
    HA  3.875000
    CB  30.936000
    HB1  1.388000
    HB2  1.211000
    CG  27.080000
    HG1  1.319000
    HG2  1.173000
    CD  43.052000
    HD1  2.971000
  END_RES_DEF

  RES_ID          766
```

```
 RES_TYPE         SER
 SPIN_SYSTEM_ID   52
 HETEROGENEITY    100
   N  116.600000
   HN   8.387000
   CA  54.618000
   HA   4.984000
   CB  38.640000
   HB1  3.034000
   HB2  2.907000
 END_RES_DEF

 RES_ID           767
 RES_TYPE         PRO
 SPIN_SYSTEM_ID   53
 HETEROGENEITY    100
   CA  63.429000
   HA   4.083000
   CB  32.588000
   HB1  2.209000
   CG  28.180000
   HG1  2.177000
   HG2  1.883000
   CD  50.763000
   HD2  3.390000
   HD1  3.623000
 END_RES_DEF

 RES_ID           768
 RES_TYPE         MET
 SPIN_SYSTEM_ID   54
 HETEROGENEITY    100
   N  119.060000
   HN   8.430000
   CA  54.067000
   HA   4.935000
   CB  31.487000
   HB1  1.989000
   HB2  1.353000
   CG  30.930000
   HG1  2.690000
   CE  14.414000
   HE#  1.929000
 END_RES_DEF

 RES_ID           769
 RES_TYPE         ASP
 SPIN_SYSTEM_ID   55
 HETEROGENEITY    100
   N  119.060000
   HN   7.365000
   CA  53.516000
   HA   4.745000
   CB  44.154000
   HB1  2.371000
 END_RES_DEF

 RES_ID           770
 RES_TYPE         LEU
 SPIN_SYSTEM_ID   56
 HETEROGENEITY    100
   N  116.272000
   HN   9.055000
   CA  57.922000
   HA   4.036000
   CB  41.400000
   HB1  2.095000
   HB2  1.395000
   CG  27.080000
   HG   1.713000
   CD1  27.080000
   HD1#  0.940000
   CD2  22.675000
   HD2#  0.628000
 END_RES_DEF

 RES_ID           771
 RES_TYPE         LYS
 SPIN_SYSTEM_ID   57
 HETEROGENEITY    100
   N  128.079000
   HN   8.738000
   CA  60.676000
   HA   4.198000
   CB  32.037000
   HB1  2.330000
   HB2  2.224000
   CG  25.280000
   HG1  1.483000
   HG2  1.403000
   CD  30.385000
   HD1  1.793000
   HD2  1.696000
   CE  41.950000
   HE1  2.965000
 END_RES_DEF

 RES_ID           772
 RES_TYPE         THR
 SPIN_SYSTEM_ID   58
 HETEROGENEITY    100
   N  122.176000
   HN   9.445000
   CA  67.040000
   HA   3.845000
   CB  67.835000
   HB   4.090000
   CG2  22.124000
   HG2#  1.058000
 END_RES_DEF

 RES_ID           773
 RES_TYPE         MET
 SPIN_SYSTEM_ID   59
 HETEROGENEITY    100
   N  117.912000
   HN   7.882000
   CA  60.676000
   HA   4.319000
   CB  33.342000
   HB1  2.093000
   HB2  1.915000
   CG  33.139000
   HG1  2.621000
   HG2  2.496000
   CE  16.620000
   HE#  1.241000
 END_RES_DEF

 RES_ID           774
 RES_TYPE         SER
 SPIN_SYSTEM_ID   60
 HETEROGENEITY    100
   N  116.108000
   HN   7.958000
   CA  62.879000
   HA   4.200000
   CB  62.879000
   HB1  4.368000
   HB2  4.040000
 END_RES_DEF

 RES_ID           775
 RES_TYPE         GLU
 SPIN_SYSTEM_ID   61
 HETEROGENEITY    100
   N  124.471000
   HN   8.150000
   CA  59.570000
   HA   4.045000
   CB  29.280000
   HB1  2.246000
   HB2  2.063000
   CG  36.443000
   HG1  2.345000
   HG2  2.176000
 END_RES_DEF

 RES_ID           776
 RES_TYPE         ARG
 SPIN_SYSTEM_ID   62
 HETEROGENEITY    100
   N  120.372000
   HN   8.391000
   CA  60.676000
   HA   3.869000
   CB  30.385000
   HB1  2.047000
   HB2  1.076000
   CG  29.284000
   HG1  1.722000
   HG2  0.877000
   CD  44.154000
   HD1  2.578000
   HD2  2.051000
 END_RES_DEF

 RES_ID           777
 RES_TYPE         LEU
 SPIN_SYSTEM_ID   63
 HETEROGENEITY    100
   N  120.208000
   HN   8.856000
   CA  58.470000
   HA   4.691000
   CB  42.621000
   HB1  2.295000
   HB2  1.925000
   CG  27.080000
   HG   1.832000
   CD1  25.429000
   HD1#  1.067000
   CD2  27.081000
   HD2#  0.871000
 END_RES_DEF

 RES_ID           778
 RES_TYPE         LYS
 SPIN_SYSTEM_ID   64
 HETEROGENEITY    100
   N  120.372000
   HN   7.958000
   CA  59.574000
   HA   4.333000
   CB  32.588000
   HB1  2.055000
   CG  24.878000
   HG1  1.596000
   CD  29.835000
   HD1  1.804000
   CE  41.951000
   HE1  2.990000
 END_RES_DEF

 RES_ID           779
 RES_TYPE         ASN
 SPIN_SYSTEM_ID   65
 HETEROGENEITY    100
   N  116.108000
   HN   7.947000
   CA  53.510000
   HA   4.771000
   CB  38.095000
   HB1  3.019000
   HB2  2.773000
   ND2  112.665000
   HD21  7.598000
   HD22  6.969000
 END_RES_DEF

 RES_ID           780
 RES_TYPE         ARG
 SPIN_SYSTEM_ID   66
 HETEROGENEITY    100
   N  114.141000
   HN   8.158000
   CA  56.821000
   HA   4.405000
   CB  25.429000
   HB1  2.097000
   HB2  2.022000
   CG  27.632000
   HG1  1.539000
   HG2  1.534000
   CD  43.050000
   HD1  3.060000
   HD2  3.024000
 END_RES_DEF

 RES_ID           781
 RES_TYPE         TYR
 SPIN_SYSTEM_ID   67
 HETEROGENEITY    100
   N  116.764000
   HN   8.222000
   CA  60.125000
   HA   4.064000
   CB  40.850000
   HB1  2.948000
   HB2  2.055000
   CD1  134.350000
   HD1  6.285000
   CE1  118.930000
   HE1  6.709000
 END_RES_DEF

 RES_ID           782
 RES_TYPE         TYR
 SPIN_SYSTEM_ID   68
 HETEROGENEITY    100
   N  114.633000
   HN   8.014000
   CA  57.920000
   HA   4.528000
   CB  36.443000
   HB1  3.062000
   HB2  2.907000
   CD1  133.248000
   HD1  7.175000
   CE1  120.582000
   HE1  7.286000
 END_RES_DEF

 RES_ID           783
 RES_TYPE         VAL
 SPIN_SYSTEM_ID   69
 HETEROGENEITY    100
   N  115.780000
   HN   7.698000
   CA  62.330000
   HA   4.083000
   CB  31.500000
   HB   2.321000
   CG1  21.570000
   HG1#  0.944000
   CG2  18.820000
   HG2#  0.823000
 END_RES_DEF

 RES_ID           784
 RES_TYPE         SER
 SPIN_SYSTEM_ID   70
 HETEROGENEITY    100
   N  111.353000
   HN   7.415000
   CA  55.719000
   HA   4.741000
   CB  66.183000
   HB1  4.200000
   HB2  3.750000
 END_RES_DEF

 RES_ID           785
 RES_TYPE         LYS
 SPIN_SYSTEM_ID   71
 HETEROGENEITY    100
   CA  59.030000
   HA   4.021000
   CB  31.590000
 END_RES_DEF

 RES_ID           786
 RES_TYPE         LYS
 SPIN_SYSTEM_ID   72
 HETEROGENEITY    100
   N  120.208000
   HN   8.244000
   CA  59.720000
   HA   4.062000
   CB  30.385000
   HB1  1.779000
   CG  24.530000
   CD  28.182000
   HD1  1.680000
   CE  41.670000
   HE1  3.137000
   HE2  3.045000
 END_RES_DEF

 RES_ID           787
 RES_TYPE         LEU
 SPIN_SYSTEM_ID   73
 HETEROGENEITY    100
   N  118.732000
   HN   7.422000
   CA  57.922000
   HA   4.213000
   CB  43.603000
   HB1  1.996000
   HB2  1.891000
   CG  27.632000
   HG   1.794000
   CD1  25.979000
   HD1#  0.924000
   CD2  23.776000
   HD2#  0.895000
 END_RES_DEF

 RES_ID           788
 RES_TYPE         PHE
 SPIN_SYSTEM_ID   74
 HETEROGENEITY    100
   N  118.732000
   HN   6.928000
   CA  60.676000
   HA   3.763000
   CB  39.750000
   HB1  2.945000
   HB2  2.381000
   CD1  133.799000
   HD1  6.400000
   CE1  131.596000
   HE1  6.928000
 END_RES_DEF

 RES_ID           789
 RES_TYPE         MET
 SPIN_SYSTEM_ID   75
 HETEROGENEITY    100
   N  116.272000
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    HN   8.489000
    CA  59.020000
    HA   3.911000
    CB  32.590000
    HB1  2.318000
    HB2  2.208000
    CG  33.140000
    HG1  2.942000
    HG2  2.611000
    CE  17.168000
    HE#  2.027000
  END_RES_DEF

  RES_ID           790
  RES_TYPE         ALA
  SPIN_SYSTEM_ID   76
  HETEROGENEITY    100
    N  119.716000
    HN   8.000000
    CA  55.170000
    HA   4.084000
    CB  18.270000
    HB#  1.485000
  END_RES_DEF

  RES_ID           791
  RES_TYPE         ASP
  SPIN_SYSTEM_ID   77
  HETEROGENEITY    100
    N  119.716000
    HN   7.376000
    CA  57.371000
    HA   4.371000
    CB  38.646000
    HB1  2.730000
  END_RES_DEF

  RES_ID           792
  RES_TYPE         LEU
  SPIN_SYSTEM_ID   78
  HETEROGENEITY    100
    N  119.550000
    HN   7.363000
    CA  57.922000
    HA   3.398000
    CB  40.299000
    HB1  0.757000
    HB2  0.442000
    CG  27.632000
    HG   0.707000
    CD1 24.327000
    HD1# 0.184000
    CD2 25.979000
    HD2# 0.061000
  END_RES_DEF

  RES_ID           793
  RES_TYPE         GLN
  SPIN_SYSTEM_ID   79
  HETEROGENEITY    100
    N  114.141000
    HN   8.069000
    CA  59.024000
    HA   3.804000
    CB  28.733000
    HB1  2.157000
    HB2  2.097000
    CG  35.342000
    HG1  2.460000
    NE2 111.353000
    HE21 7.319000
    HE22 7.222000
  END_RES_DEF

  RES_ID           794
  RES_TYPE         ARG
  SPIN_SYSTEM_ID   80
  HETEROGENEITY    100
    N  118.568000
    HN   7.382000
    CA  58.473000
    HA   4.078000
    CB  29.835000
    HB1  1.973000
    HB2  1.886000
    CG  27.080000
    HG1  1.742000
    CD  43.603000
    HD1  3.390000
    HD2  3.325000
  END_RES_DEF

  RES_ID           795
  RES_TYPE         VAL
  SPIN_SYSTEM_ID   81
  HETEROGENEITY    100
    N  117.912000
    HN   7.013000
    CA  66.730000
    HA   3.039000
    CB  30.930000
    HB   1.435000
    CG1 22.124000
    HG1# 0.479000
    CG2 21.573000
    HG2# 0.142000
  END_RES_DEF

  RES_ID           796
  RES_TYPE         PHE
  SPIN_SYSTEM_ID   82
  HETEROGENEITY    100
    N  116.928000
    HN   6.357000
    CA  58.470000
    HA   4.161000
    CB  38.096000
    HB1  3.090000
    HB2  2.944000
    CD1 132.147000
    HD1  6.641000
    CE1 131.596000
    HE1  6.456000
    CZ  129.393000
    HZ   6.406000
  END_RES_DEF

  RES_ID           797
  RES_TYPE         THR
  SPIN_SYSTEM_ID   83
  HETEROGENEITY    100
    N  115.289000
    HN   9.047000
    CA  66.734000
    HA   3.838000
    CB  68.380000
    HB   4.210000
    CG2 22.120000
    HG2# 1.296000
  END_RES_DEF

  RES_ID           798
  RES_TYPE         ASN
  SPIN_SYSTEM_ID   84
  HETEROGENEITY    100
    N  120.700000
    HN   8.846000
    CA  55.170000
    HA   4.315000
    CB  38.090000
    HB1  2.985000
    HB2  2.661000
  END_RES_DEF

  RES_ID           799
  RES_TYPE         CYS
  SPIN_SYSTEM_ID   85
  HETEROGENEITY    100
    N  116.928000
    HN   6.893000
    CA  62.157000
    HA   4.405000
    CB  26.530000
    HB1  3.304000
    HB2  3.032000
  END_RES_DEF

  RES_ID           800
  RES_TYPE         LYS
  SPIN_SYSTEM_ID   86
  HETEROGENEITY    100
    N  116.764000
    HN   7.799000
    CA  58.473000
    HA   4.204000
    CB  32.588000
    HB1  1.743000
    CG  25.429000
    HG1  1.313000
    HG2  0.138000
    CD  29.835000
    HD1  1.291000
    CE  41.400000
    HE1  2.486000
    HE2  2.421000
  END_RES_DEF

  RES_ID           801
  RES_TYPE         GLU
  SPIN_SYSTEM_ID   87
  HETEROGENEITY    100
    N  117.912000
    HN   7.945000
    CA  57.992000
    HA   4.250000
    CB  30.385000
    HB1  2.172000
    HB2  2.003000
    CG  36.994000
    HG1  2.407000
    HG2  2.203000
  END_RES_DEF

  RES_ID           802
  RES_TYPE         TYR
  SPIN_SYSTEM_ID   88
  HETEROGENEITY    100
    N  116.600000
    HN   7.744000
    CA  60.676000
    HA   4.369000
    CB  41.400000
    HB1  2.929000
    CD1 134.901000
    HD1  6.989000
    CE1 119.481000
    HE1  6.823000
  END_RES_DEF

  RES_ID           803
  RES_TYPE         ASN
  SPIN_SYSTEM_ID   89
  HETEROGENEITY    100
    N  115.944000
    HN   8.241000
    CA  51.864000
    HA   5.024000
    CB  40.849000
    HB1  3.069000
    HB2  2.907000
    ND2 118.732000
    HD21 8.316000
    HD22 7.809000
  END_RES_DEF

  RES_ID           804
  RES_TYPE         ALA
  SPIN_SYSTEM_ID   90
  HETEROGENEITY    100
  END_RES_DEF

  RES_ID           805
  RES_TYPE         PRO
  SPIN_SYSTEM_ID   91
  HETEROGENEITY    100
    CA  63.980000
    HA   2.422000
    HB1  1.949000
    HG1  1.648000
    HG2  1.558000
    CD  50.762000
    HD2  3.601000
    HD1  3.706000
  END_RES_DEF

  RES_ID           806
  RES_TYPE         GLU
  SPIN_SYSTEM_ID   92
  HETEROGENEITY    100
    N  112.993000
    HN   8.246000
    CA  56.820000
    HA   4.185000
    CB  28.733000
    HB1  2.095000
    HB2  1.973000
    CG  36.270000
    HG1  2.200000
  END_RES_DEF

  RES_ID           807
  RES_TYPE         SER
  SPIN_SYSTEM_ID   93
  HETEROGENEITY    100
    N  115.780000
    HN   8.112000
    CA  58.473000
    HA   4.406000
    CB  66.183000
    HB1  4.393000
    HB2  4.157000
  END_RES_DEF

  RES_ID           808
  RES_TYPE         GLU
  SPIN_SYSTEM_ID   94
  HETEROGENEITY    100
    N  123.488000
    HN   9.061000
    CA  59.574000
    HA   4.232000
    CB  29.835000
    HB1  2.169000
    CG  36.443000
    HG1  2.528000
  END_RES_DEF

  RES_ID           809
  RES_TYPE         TYR
  SPIN_SYSTEM_ID   95
  HETEROGENEITY    100
    N  116.436000
    HN   8.072000
    CA  60.120000
    HA   3.834000
    CB  37.550000
    HB1  3.018000
    HB2  2.738000
    CD1 132.698000
    HD1  6.891000
    CE1 120.032000
    HE1  7.011000
  END_RES_DEF

  RES_ID           810
  RES_TYPE         TYR
  SPIN_SYSTEM_ID   96
  HETEROGENEITY    100
    N  119.880000
    HN   7.356000
    CA  61.777000
    HA   3.819000
    CB  40.300000
    HB1  3.390000
    HB2  2.500000
    CD1 136.553000
    HD1  7.094000
    CE1 119.481000
    HE1  7.000000
  END_RES_DEF

  RES_ID           811
  RES_TYPE         LYS
  SPIN_SYSTEM_ID   97
  HETEROGENEITY    100
    N  118.076000
    HN   8.072000
    CA  60.676000
    HA   4.204000
    CB  32.588000
    HB1  2.091000
    CG  25.979000
    HG1  1.819000
    HG2  1.582000
    CD  29.834000
    HD1  1.813000
    CE  41.963000
    HE1  2.962000
  END_RES_DEF

  RES_ID           812
  RES_TYPE         CYS
  SPIN_SYSTEM_ID   98
  HETEROGENEITY    100
    N  116.764000
    HN   8.520000
    CA  65.087000
    HA   4.202000
    CB  27.080000
    HB1  3.396000
    HB2  3.056000
  END_RES_DEF

  RES_ID           813
  RES_TYPE         ALA
  SPIN_SYSTEM_ID   99
  HETEROGENEITY    100
    N  120.700000
    HN   8.315000
    CA  55.563000
    HA   3.834000
    CB  18.270000
    HB#  1.597000
  END_RES_DEF

  RES_ID           814
  RES_TYPE         ASN
  SPIN_SYSTEM_ID   100
  HETEROGENEITY    100
    N  115.453000
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```
    HN   8.068000
    CA  56.270000
    HA   4.329000
    CB  38.646000
    HB1  2.877000
    HB2  2.834000
  END_RES_DEF

  RES_ID           815
  RES_TYPE         ILE
  SPIN_SYSTEM_ID   101
  HETEROGENEITY    100
    N  119.880000
    HN   7.912000
    CA  65.080000
    HA   3.646000
    CB  39.197000
    HB   1.924000
    CG1  29.284000
    HG11  1.882000
    HG12  1.201000
    CG2  17.718000
    HG2#  1.017000
    CD1  13.863000
    HD1#  0.940000
  END_RES_DEF

  RES_ID           816
  RES_TYPE         LEU
  SPIN_SYSTEM_ID   102
  HETEROGENEITY    100
    N  122.504000
    HN   8.556000
    CA  56.820000
    HA   3.670000
    CB  41.951000
    HB1  1.405000
    HB2  1.199000
    CG  26.530000
    HG   1.580000
    CD1  24.327000
    HD1#  0.701000
    CD2  25.429000
    HD2#  0.696000
  END_RES_DEF

  RES_ID           817
  RES_TYPE         GLU
  SPIN_SYSTEM_ID   103
  HETEROGENEITY    100
    N  120.700000
    HN   8.073000
    CA  60.125000
    HA   3.185000
    CB  29.835000
    HB1  1.720000
    HB2  1.310000
    CG  37.545000
    HG1  2.001000
    HG2  1.922000
  END_RES_DEF

  RES_ID           818
  RES_TYPE         LYS
  SPIN_SYSTEM_ID   104
  HETEROGENEITY    100
    N  117.584000
    HN   7.145000
    CA  59.688000
    HA   4.075000
    CB  32.588000
    HB1  1.929000
    CG  25.644000
    HG1  1.492000
    CD  29.284000
    HD1  1.681000
    CE  41.963000
    HE1  2.964000
  END_RES_DEF

  RES_ID           819
  RES_TYPE         PHE
  SPIN_SYSTEM_ID   105
  HETEROGENEITY    100
    N  121.028000
    HN   7.869000
    CA  61.230000
    HA   4.328000
    CB  39.200000
    HB1  3.133000
    HB2  3.047000
    CD1  133.800000
    HD1  7.180000
  END_RES_DEF

  RES_ID           820
  RES_TYPE         PHE
  SPIN_SYSTEM_ID   106
  HETEROGENEITY    100
    N  120.700000
    HN   9.126000
    CA  60.691000
    HA   3.961000
    CB  38.640000
    HB1  3.289000
    HB2  3.067000
    CD1  133.248000
    HD1  6.904000
    CE1  132.698000
    HE1  7.011000
  END_RES_DEF

  RES_ID           821
  RES_TYPE         PHE
  SPIN_SYSTEM_ID   107
  HETEROGENEITY    100
    N  118.076000
    HN   8.359000
    CA  61.770000
    HA   3.840000
    CB  38.090000
    HB1  3.064000
    CD1  133.248000
    HD1  7.175000
    CE1  132.698000
    HE1  7.294000
    CZ  131.596000
    HZ   7.430000
  END_RES_DEF

  RES_ID           822
  RES_TYPE         SER
  SPIN_SYSTEM_ID   108
  HETEROGENEITY    100
    N  114.961000
    HN   7.906000
    CA  61.773000
    HA   4.200000
    CB  62.879000
    HB1  4.007000
  END_RES_DEF

  RES_ID           823
  RES_TYPE         LYS
  SPIN_SYSTEM_ID   109
  HETEROGENEITY    100
    N  120.864000
    HN   7.938000
    CA  56.820000
    HA   4.008000
    CB  31.487000
    HB1  1.730000
    HB2  1.567000
    CG  23.226000
    HG1  0.833000
    CD  27.080000
    HD1  1.403000
    CE  42.501000
    HE1  2.569000
    HE2  2.422000
  END_RES_DEF

  RES_ID           824
  RES_TYPE         ILE
  SPIN_SYSTEM_ID   110
  HETEROGENEITY    100
    N  116.928000
    HN   8.101000
    CA  64.530000
    HA   3.818000
    CB  36.990000
    HB   1.746000
    CG1  26.530000
    HG11  1.140000
    HG12  1.073000
    CG2  18.820000
    HG2#  0.654000
    CD1  13.312000
    HD1#  0.541000
  END_RES_DEF

  RES_ID           825
  RES_TYPE         LYS
  SPIN_SYSTEM_ID   111
  HETEROGENEITY    100
    N  122.176000
    HN   7.546000
    CA  59.024000
    HA   4.043000
    CB  32.360000
    HB1  1.879000
    HB2  1.757000
    CG  24.878000
    HG1  1.390000
    HG2  1.302000
    CD  29.284000
    HD1  1.633000
    CE  41.400000
    HE1  2.913000
  END_RES_DEF

  RES_ID           826
  RES_TYPE         GLU
  SPIN_SYSTEM_ID   112
  HETEROGENEITY    100
    N  121.192000
    HN   8.063000
    CA  59.024000
    HA   3.995000
    CB  29.834000
    HB1  2.058000
    CG  36.050000
    HG1  2.342000
    HG2  2.205000
  END_RES_DEF

  RES_ID           827
  RES_TYPE         ALA
  SPIN_SYSTEM_ID   113
  HETEROGENEITY    100
    N  117.748000
    HN   7.620000
    CA  52.410000
    HA   4.291000
    CB  19.920000
    HB#  1.358000
  END_RES_DEF

  RES_ID           828
  RES_TYPE         GLY
  SPIN_SYSTEM_ID   114
  HETEROGENEITY    100
    N  126.767000
    HN   7.744000
    CA  45.902000
    HA1  4.019000
    HA2  3.935000
  END_RES_DEF

  RES_ID           829
  RES_TYPE         LEU
  SPIN_SYSTEM_ID   115
  HETEROGENEITY    100
    N  117.912000
    HN   7.742000
    CA  55.719000
    HA   4.215000
    CB  43.052000
    HB1  1.562000
    CG  27.632000
    HG   1.536000
    CD1  23.776000
    HD1#  0.711000
  END_RES_DEF

  RES_ID           830
  RES_TYPE         ILE
  SPIN_SYSTEM_ID   116
  HETEROGENEITY    100
    N  115.453000
    HN   7.458000
    CA  60.676000
    HA   4.232000
    CB  39.748000
    HB   1.810000
    CG1  27.080000
    HG11  1.314000
    HG12  0.918000
    CG2  17.718000
    HG2#  0.815000
    CD1  13.312000
    HD1#  0.794000
  END_RES_DEF

  RES_ID           831
  RES_TYPE         ASP
  SPIN_SYSTEM_ID   117
  HETEROGENEITY    100
    N  123.488000
    HN   8.270000
    CA  54.620000
    HA   4.571000
    CB  41.400000
    HB1  2.693000
    HB2  2.540000
  END_RES_DEF

  RES_ID           832
  RES_TYPE         LYS
  SPIN_SYSTEM_ID   118
  HETEROGENEITY    100
    N  125.450000
    HN   7.774000
    CA  57.720000
    HA   4.082000
    CB  33.410000
  END_RES_DEF
```

Table 2

Unambiguous NOE-derived Inter-proton Distance Restraints

```
ASSI ( 2141)
   (( segid "BrD " and resid 89   and name HN  ))
   ( segid "BrD " and resid 96   and name HD% )
     4.200     4.200     1.300 peak  2141 weight  0.11000E+01 volume  0.36756E+02 ppm1      8.857 ppm2      7.704
 ASSI (13261)
   (( segid "BrD " and resid 89   and name HD22))
   ( segid "BrD " and resid 95   and name HE% )
     3.900     3.800     1.600 peak 13261 weight  0.11000E+01 volume  0.50220E+02 ppm1      8.416 ppm2      7.624
 ASSI (13271)
   (( segid "BrD " and resid 89   and name HD21))
   ( segid "BrD " and resid 95   and name HE% )
     4.000     4.000     1.500 peak 13271 weight  0.11000E+01 volume  0.43992E+02 ppm1      8.924 ppm2      7.624
 ASSI ( 6521)
   (( segid "BrD " and resid 46   and name HN  ))
   ( segid "BrD " and resid 47   and name HD% )
     3.500     3.100     2.000 peak  6521 weight  0.11000E+01 volume  0.10017E+03 ppm1      8.562 ppm2      7.960
 ASSI (14401)
   (( segid "BrD " and resid 87   and name HN  ))
   (( segid "BrD " and resid 88   and name HB1 ))
     3.700     3.400     1.800 peak 14401 weight  0.11000E+01 volume  0.72183E+02 ppm1      8.572 ppm2      3.532
  OR (14401)
   (( segid "BrD " and resid 87   and name HN  ))
   (( segid "BrD " and resid 88   and name HB2 ))
 ASSI (15611)
   (( segid "BrD " and resid 32   and name HE1 ))
   (( segid "BrD " and resid 94   and name HG2 ))
     4.500     4.500     1.000 peak 15611 weight  0.11000E+01 volume  0.23846E+02 ppm1     11.082 ppm2      3.143
  OR (15611)
   (( segid "BrD " and resid 32   and name HE1 ))
   (( segid "BrD " and resid 94   and name HG1 ))
 ASSI (    1)
   (( segid "BrD " and resid 43   and name HN  ))
   (( segid "BrD " and resid 43   and name HA  ))
     2.700     1.800     1.800 peak     1 weight  0.11000E+01 volume  0.52965E+03 ppm1      8.001 ppm2      5.544
 ASSI (   11)
   (( segid "BrD " and resid 43   and name HN  ))
   ( segid "BrD " and resid 43   and name HB% )
     2.400     1.400     1.400 peak    11 weight  0.11000E+01 volume  0.93421E+03 ppm1      8.001 ppm2      1.689
 ASSI (   21)
   (( segid "BrD " and resid 43   and name HN  ))
   (( segid "BrD " and resid 42   and name HN  ))
     2.200     1.200     1.200 peak    21 weight  0.11000E+01 volume  0.18953E+04 ppm1      8.001 ppm2      7.816
 ASSI (   31)
   (( segid "BrD " and resid 42   and name HN  ))
   (( segid "BrD " and resid 41   and name HB  ))
     3.300     2.700     2.200 peak    31 weight  0.11000E+01 volume  0.14380E+03 ppm1      7.822 ppm2      4.900
 ASSI (   41)
   (( segid "BrD " and resid 42   and name HN  ))
   (( segid "BrD " and resid 42   and name HA  ))
     2.900     2.100     2.100 peak    41 weight  0.11000E+01 volume  0.30790E+03 ppm1      7.824 ppm2      5.053
 ASSI (   51)
   (( segid "BrD " and resid 42   and name HN  ))
   (( segid "BrD " and resid 42   and name HB2 ))
     2.700     1.800     1.800 peak    51 weight  0.11000E+01 volume  0.47343E+03 ppm1      7.821 ppm2      2.613
 ASSI (   61)
   (( segid "BrD " and resid 42   and name HN  ))
   (( segid "BrD " and resid 42   and name HG1 ))
     3.200     2.600     2.300 peak    61 weight  0.11000E+01 volume  0.16643E+03 ppm1      7.822 ppm2      2.899
 ASSI (   71)
   (( segid "BrD " and resid 42   and name HN  ))
   (( segid "BrD " and resid 42   and name HB1 ))
     3.400     2.900     2.100 peak    71 weight  0.11000E+01 volume  0.13090E+03 ppm1      7.821 ppm2      2.790
 ASSI (   91)
   (( segid "BrD " and resid 99   and name HN  ))
   ( segid "BrD " and resid 99   and name HB% )
     2.400     1.400     1.400 peak    91 weight  0.11000E+01 volume  0.90687E+03 ppm1      8.936 ppm2      2.208
 ASSI (  101)
   (( segid "BrD " and resid 99   and name HN  ))
   (( segid "BrD " and resid 99   and name HA  ))
     2.800     2.000     2.000 peak   101 weight  0.11000E+01 volume  0.42952E+03 ppm1      8.936 ppm2      4.441
 ASSI (  121)
   (( segid "BrD " and resid 99   and name HN  ))
   (( segid "BrD " and resid 98   and name HN  ))
     2.700     1.800     1.800 peak   121 weight  0.11000E+01 volume  0.45502E+03 ppm1      8.936 ppm2      9.112
 ASSI (  131)
   (( segid "BrD " and resid 98   and name HN  ))
   (( segid "BrD " and resid 98   and name HA  ))
     2.500     1.600     1.600 peak   131 weight  0.11000E+01 volume  0.72592E+03 ppm1      9.125 ppm2      4.811
 ASSI (  141)
   (( segid "BrD " and resid 98   and name HN  ))
   (( segid "BrD " and resid 98   and name HB1 ))
     3.300     2.700     2.200 peak   141 weight  0.11000E+01 volume  0.15487E+03 ppm1      9.125 ppm2      4.010
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ASSI ( 151)
   (( segid "BrD " and resid 98   and name HN  ))
   (( segid "BrD " and resid 98   and name HB2 ))
     2.400     1.400     1.400 peak   151 weight  0.11000E+01 volume  0.95273E+03 ppm1      9.125 ppm2      3.656
 ASSI ( 171)
   (( segid "BrD " and resid 30   and name HN  ))
   (( segid "BrD " and resid 30   and name HA  ))
     3.100     2.400     2.400 peak   171 weight  0.11000E+01 volume  0.20628E+03 ppm1     12.275 ppm2      5.451
 ASSI ( 181)
   (( segid "BrD " and resid 30   and name HN  ))
   (( segid "BrD " and resid 30   and name HB1 ))
     3.200     2.600     2.300 peak   181 weight  0.11000E+01 volume  0.16806E+03 ppm1     12.275 ppm2      4.939
 ASSI ( 191)
   (( segid "BrD " and resid 30   and name HN  ))
   (( segid "BrD " and resid 30   and name HB2 ))
     2.800     2.000     2.000 peak   191 weight  0.11000E+01 volume  0.40863E+03 ppm1     12.275 ppm2      4.538
 ASSI ( 201)
   (( segid "BrD " and resid 30   and name HN  ))
   (( segid "BrD " and resid 29   and name HN  ))
     3.300     2.700     2.200 peak   201 weight  0.11000E+01 volume  0.15134E+03 ppm1     12.275 ppm2      9.150
 ASSI ( 211)
   (( segid "BrD " and resid 29   and name HN  ))
   (( segid "BrD " and resid 29   and name HA  ))
     2.700     1.800     1.800 peak   211 weight  0.11000E+01 volume  0.44644E+03 ppm1      9.151 ppm2      4.818
 ASSI ( 221)
   (( segid "BrD " and resid 29   and name HN  ))
   (( segid "BrD " and resid 29   and name HB1 ))
     2.800     2.000     2.000 peak   221 weight  0.11000E+01 volume  0.39478E+03 ppm1      9.152 ppm2      2.712
 ASSI ( 231)
   (( segid "BrD " and resid 31   and name HN  ))
   (( segid "BrD " and resid 29   and name HA  ))
     3.400     2.900     2.100 peak   231 weight  0.11000E+01 volume  0.12405E+03 ppm1      8.479 ppm2      4.816
 ASSI ( 241)
   (( segid "BrD " and resid 31   and name HN  ))
   (( segid "BrD " and resid 31   and name HA  ))
     3.300     2.700     2.200 peak   241 weight  0.11000E+01 volume  0.13933E+03 ppm1      8.479 ppm2      5.003
 ASSI ( 251)
   (( segid "BrD " and resid 31   and name HN  ))
   ( segid "BrD " and resid 31   and name HB% )
     2.400     1.400     1.400 peak   251 weight  0.11000E+01 volume  0.88455E+03 ppm1      8.480 ppm2      2.307
 ASSI ( 271)
   (( segid "BrD " and resid 28   and name HN  ))
   (( segid "BrD " and resid 28   and name HB2 ))
     2.500     1.600     1.600 peak   271 weight  0.11000E+01 volume  0.82952E+03 ppm1      8.166 ppm2      3.409
 ASSI ( 281)
   (( segid "BrD " and resid 28   and name HN  ))
   (( segid "BrD " and resid 28   and name HB1 ))
     2.500     1.600     1.600 peak   281 weight  0.11000E+01 volume  0.71832E+03 ppm1      8.166 ppm2      3.596
 ASSI ( 291)
   (( segid "BrD " and resid 28   and name HN  ))
   (( segid "BrD " and resid 28   and name HA  ))
     2.700     1.800     1.800 peak   291 weight  0.11000E+01 volume  0.53058E+03 ppm1      8.165 ppm2      4.598
 ASSI ( 301)
   (( segid "BrD " and resid 28   and name HN  ))
   (( segid "BrD " and resid 29   and name HN  ))
     3.400     2.900     2.100 peak   301 weight  0.11000E+01 volume  0.11688E+03 ppm1      8.166 ppm2      9.164
 ASSI ( 321)
   (( segid "BrD " and resid 32   and name HN  ))
   (( segid "BrD " and resid 32   and name HA  ))
     2.600     1.700     1.700 peak   321 weight  0.11000E+01 volume  0.66621E+03 ppm1      7.739 ppm2      4.977
 ASSI ( 331)
   (( segid "BrD " and resid 32   and name HN  ))
   (( segid "BrD " and resid 32   and name HB1 ))
     2.900     2.100     2.100 peak   331 weight  0.11000E+01 volume  0.30872E+03 ppm1      7.740 ppm2      4.201
 ASSI ( 341)
   (( segid "BrD " and resid 32   and name HN  ))
   (( segid "BrD " and resid 32   and name HB2 ))
     2.600     1.700     1.700 peak   341 weight  0.11000E+01 volume  0.59972E+03 ppm1      7.739 ppm2      3.958
 ASSI ( 351)
   (( segid "BrD " and resid 30   and name HN  ))
   (( segid "BrD " and resid 31   and name HN  ))
     2.800     2.000     2.000 peak   351 weight  0.11000E+01 volume  0.41861E+03 ppm1     12.275 ppm2      8.477
 ASSI ( 361)
   (( segid "BrD " and resid 105  and name HN  ))
   (( segid "BrD " and resid 105  and name HA  ))
     3.100     2.400     2.400 peak   361 weight  0.11000E+01 volume  0.32043E+03 ppm1      8.488 ppm2      4.934
 ASSI ( 371)
   (( segid "BrD " and resid 105  and name HN  ))
   (( segid "BrD " and resid 105  and name HB1 ))
     2.800     2.000     2.000 peak   371 weight  0.11000E+01 volume  0.42542E+03 ppm1      8.487 ppm2      3.740
 ASSI ( 401)
   (( segid "BrD " and resid 106  and name HN  ))
   (( segid "BrD " and resid 105  and name HN  ))
     2.700     1.800     1.800 peak   401 weight  0.11000E+01 volume  0.44987E+03 ppm1      9.740 ppm2      8.476
 ASSI ( 411)
   (( segid "BrD " and resid 106  and name HN  ))
   (( segid "BrD " and resid 106  and name HA  ))
     2.600     1.700     1.700 peak   411 weight  0.11000E+01 volume  0.55394E+03 ppm1      9.740 ppm2      4.566
 ASSI ( 421)
   (( segid "BrD " and resid 106  and name HN  ))
   (( segid "BrD " and resid 106  and name HB1 ))
     2.500     1.600     1.600 peak   421 weight  0.11000E+01 volume  0.71868E+03 ppm1      9.740 ppm2      3.895
 ASSI ( 431)
   (( segid "BrD " and resid 106  and name HN  ))
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   (( segid "BrD " and resid 106  and name HB2 ))
     2.300      1.300      1.300 peak   431 weight  0.11000E+01 volume  0.11998E+04 ppm1      9.740 ppm2      3.674
ASSI [  451]
   (( segid "BrD " and resid 107  and name HN  ))
   (( segid "BrD " and resid 106  and name HN  ))
     2.900      2.100      2.100 peak   451 weight  0.11000E+01 volume  0.34881E+03 ppm1      8.981 ppm2      9.713
ASSI [  461]
   (( segid "BrD " and resid 107  and name HN  ))
   ( segid "BrD " and resid 107  and name HD% )
     3.500      3.100      2.000 peak   461 weight  0.11000E+01 volume  0.11255E+03 ppm1      8.980 ppm2      7.783
ASSI [  471]
   (( segid "BrD " and resid 107  and name HN  ))
   (( segid "BrD " and resid 107  and name HA  ))
     2.600      1.700      1.700 peak   471 weight  0.11000E+01 volume  0.57631E+03 ppm1      8.981 ppm2      4.443
ASSI [  481]
   (( segid "BrD " and resid 107  and name HN  ))
   (( segid "BrD " and resid 107  and name HB1 ))
     3.200      2.600      2.300 peak   481 weight  0.11000E+01 volume  0.16715E+03 ppm1      8.980 ppm2      3.671
ASSI [  501]
   (( segid "BrD " and resid 108  and name HN  ))
   (( segid "BrD " and resid 107  and name HN  ))
     2.600      1.700      1.700 peak   501 weight  0.11000E+01 volume  0.57313E+03 ppm1      8.529 ppm2      8.966
ASSI [  511]
   (( segid "BrD " and resid 108  and name HN  ))
   (( segid "BrD " and resid 108  and name HA  ))
     2.700      1.800      1.800 peak   511 weight  0.11000E+01 volume  0.52916E+03 ppm1      8.526 ppm2      4.811
ASSI [  521]
   (( segid "BrD " and resid 108  and name HN  ))
   (( segid "BrD " and resid 108  and name HB1 ))
     2.400      1.400      1.400 peak   521 weight  0.11000E+01 volume  0.97994E+03 ppm1      8.526 ppm2      4.583
ASSI [  531]
   (( segid "BrD " and resid 109  and name HN  ))
   (( segid "BrD " and resid 109  and name HA  ))
     2.300      1.300      1.300 peak   531 weight  0.11000E+01 volume  0.11922E+04 ppm1      8.572 ppm2      4.615
ASSI [  541]
   (( segid "BrD " and resid 110  and name HN  ))
   (( segid "BrD " and resid 109  and name HB2 ))
     2.900      2.100      2.100 peak   541 weight  0.11000E+01 volume  0.32815E+03 ppm1      8.714 ppm2      2.174
ASSI [  551]
   (( segid "BrD " and resid 110  and name HN  ))
   (( segid "BrD " and resid 110  and name HA  ))
     2.800      2.000      2.000 peak   551 weight  0.11000E+01 volume  0.43619E+03 ppm1      8.714 ppm2      4.451
ASSI [  561]
   (( segid "BrD " and resid 110  and name HN  ))
   (( segid "BrD " and resid 110  and name HB  ))
     2.500      1.600      1.600 peak   561 weight  0.11000E+01 volume  0.77600E+03 ppm1      8.714 ppm2      2.352
ASSI [  581]
   (( segid "BrD " and resid 109  and name HN  ))
   (( segid "BrD " and resid 110  and name HN  ))
     2.800      2.000      2.000 peak   581 weight  0.11000E+01 volume  0.41482E+03 ppm1      8.572 ppm2      8.705
ASSI [  591]
   (( segid "BrD " and resid 111  and name HN  ))
   (( segid "BrD " and resid 108  and name HA  ))
     3.200      2.600      2.300 peak   591 weight  0.11000E+01 volume  0.17690E+03 ppm1      8.168 ppm2      4.807
ASSI [  601]
   (( segid "BrD " and resid 111  and name HN  ))
   (( segid "BrD " and resid 111  and name HA  ))
     2.500      1.600      1.600 peak   601 weight  0.11000E+01 volume  0.71549E+03 ppm1      8.168 ppm2      4.650
ASSI [  621]
   (( segid "BrD " and resid 110  and name HN  ))
   (( segid "BrD " and resid 111  and name HN  ))
     2.800      2.000      2.000 peak   621 weight  0.11000E+01 volume  0.38661E+03 ppm1      8.714 ppm2      8.153
ASSI [  631]
   (( segid "BrD " and resid 112  and name HN  ))
   (( segid "BrD " and resid 112  and name HA  ))
     2.300      1.300      1.300 peak   631 weight  0.11000E+01 volume  0.13944E+04 ppm1      8.667 ppm2      4.607
ASSI [  641]
   (( segid "BrD " and resid 112  and name HN  ))
   (( segid "BrD " and resid 112  and name HG1 ))
     3.400      2.900      2.100 peak   641 weight  0.11000E+01 volume  0.12114E+03 ppm1      8.668 ppm2      2.956
ASSI [  651]
   (( segid "BrD " and resid 112  and name HN  ))
   (( segid "BrD " and resid 112  and name HG2 ))
     3.500      3.100      2.000 peak   651 weight  0.11000E+01 volume  0.96511E+02 ppm1      8.668 ppm2      2.818
ASSI [  661]
   (( segid "BrD " and resid 112  and name HN  ))
   (( segid "BrD " and resid 112  and name HB1 ))
     3.200      3.200      1.200 peak   661 weight  0.11000E+01 volume  0.15417E+04 ppm1      8.668 ppm2      2.667
ASSI [  671]
   (( segid "BrD " and resid 113  and name HN  ))
   (( segid "BrD " and resid 113  and name HA  ))
     2.800      2.000      2.000 peak   671 weight  0.11000E+01 volume  0.42878E+03 ppm1      8.217 ppm2      4.904
ASSI [  681]
   (( segid "BrD " and resid 113  and name HN  ))
   ( segid "BrD " and resid 113  and name HB% )
     2.400      1.400      1.400 peak   681 weight  0.11000E+01 volume  0.99017E+03 ppm1      8.219 ppm2      1.967
ASSI [  701]
   (( segid "BrD " and resid 114  and name HN  ))
   (( segid "BrD " and resid 114  and name HA1 ))
     2.800      2.000      2.000 peak   701 weight  0.11000E+01 volume  0.42782E+03 ppm1      8.376 ppm2      4.619
ASSI [  721]
   (( segid "BrD " and resid 113  and name HN  ))
   (( segid "BrD " and resid 114  and name HN  ))
     2.500      1.600      1.600 peak   721 weight  0.11000E+01 volume  0.73856E+03 ppm1      8.219 ppm2      8.351
ASSI [  741]
   (( segid "BrD " and resid 100  and name HN  ))
   (( segid "BrD " and resid 100  and name HA  ))
     2.700      1.800      1.800 peak   741 weight  0.11000E+01 volume  0.49224E+03 ppm1      8.669 ppm2      4.938
ASSI [  751]
   (( segid "BrD " and resid 100  and name HN  ))
   (( segid "BrD " and resid 100  and name HB2 ))
     2.400      1.400      1.400 peak   751 weight  0.11000E+01 volume  0.10916E+04 ppm1      8.669 ppm2      3.422
ASSI [  771]
   (( segid "BrD " and resid 99   and name HN  ))
   (( segid "BrD " and resid 100  and name HN  ))
     2.500      1.600      1.600 peak   771 weight  0.11000E+01 volume  0.76441E+03 ppm1      8.936 ppm2      8.664
ASSI [  791]
   (( segid "BrD " and resid 97   and name HN  ))
   (( segid "BrD " and resid 97   and name HA  ))
     2.600      1.700      1.700 peak   791 weight  0.11000E+01 volume  0.58097E+03 ppm1      8.676 ppm2      4.809
ASSI [  811]
   (( segid "BrD " and resid 97   and name HN  ))
   (( segid "BrD " and resid 98   and name HN  ))
     3.000      2.200      2.200 peak   811 weight  0.11000E+01 volume  0.25513E+03 ppm1      8.672 ppm2      9.124
ASSI [  841]
   (( segid "BrD " and resid 96   and name HN  ))
   (( segid "BrD " and resid 96   and name HA  ))
     2.600      1.700      1.700 peak   841 weight  0.11000E+01 volume  0.65098E+03 ppm1      7.977 ppm2      4.433
ASSI [  851]
   (( segid "BrD " and resid 96   and name HN  ))
   (( segid "BrD " and resid 96   and name HB1 ))
     2.800      2.000      2.000 peak   851 weight  0.11000E+01 volume  0.42091E+03 ppm1      7.976 ppm2      3.995
ASSI [  861]
   (( segid "BrD " and resid 96   and name HN  ))
   (( segid "BrD " and resid 96   and name HB2 ))
     2.600      1.700      1.700 peak   861 weight  0.11000E+01 volume  0.56648E+03 ppm1      7.979 ppm2      3.112
ASSI [  871]
   (( segid "BrD " and resid 96   and name HN  ))
   (( segid "BrD " and resid 97   and name HN  ))
     2.600      1.700      1.700 peak   871 weight  0.11000E+01 volume  0.67038E+03 ppm1      7.979 ppm2      8.678
ASSI [  891]
   (( segid "BrD " and resid 95   and name HN  ))
   (( segid "BrD " and resid 95   and name HA  ))
     3.100      2.400      2.400 peak   891 weight  0.11000E+01 volume  0.22376E+03 ppm1      8.669 ppm2      4.443
ASSI [  901]
   (( segid "BrD " and resid 95   and name HN  ))
   (( segid "BrD " and resid 95   and name HB1 ))
     2.800      2.000      2.000 peak   901 weight  0.11000E+01 volume  0.37061E+03 ppm1      8.669 ppm2      3.598
ASSI [  911]
   (( segid "BrD " and resid 95   and name HN  ))
   (( segid "BrD " and resid 95   and name HB2 ))
     2.700      1.800      1.800 peak   911 weight  0.11000E+01 volume  0.54351E+03 ppm1      8.669 ppm2      3.346
ASSI [  921]
   (( segid "BrD " and resid 94   and name HN  ))
   (( segid "BrD " and resid 94   and name HA  ))
     3.300      2.700      2.300 peak   921 weight  0.11000E+01 volume  0.13528E+03 ppm1      9.679 ppm2      4.846
ASSI [  941]
   (( segid "BrD " and resid 94   and name HN  ))
   (( segid "BrD " and resid 95   and name HN  ))
     3.500      3.100      2.000 peak   941 weight  0.11000E+01 volume  0.95054E+02 ppm1      9.679 ppm2      8.670
ASSI [  971]
   (( segid "BrD " and resid 93   and name HN  ))
   (( segid "BrD " and resid 93   and name HA  ))
     3.200      2.600      2.300 peak   971 weight  0.11000E+01 volume  0.16612E+03 ppm1      8.713 ppm2      5.037
ASSI [  981]
   (( segid "BrD " and resid 93   and name HN  ))
   (( segid "BrD " and resid 93   and name HB2 ))
     3.300      2.700      2.200 peak   981 weight  0.11000E+01 volume  0.15761E+03 ppm1      8.713 ppm2      4.753
ASSI [ 1001]
   (( segid "BrD " and resid 92   and name HN  ))
   (( segid "BrD " and resid 92   and name HA  ))
     2.500      1.600      1.600 peak  1001 weight  0.11000E+01 volume  0.71435E+03 ppm1      8.873 ppm2      4.802
ASSI [ 1011]
   (( segid "BrD " and resid 92   and name HN  ))
   (( segid "BrD " and resid 93   and name HN  ))
     2.500      1.600      1.600 peak  1011 weight  0.11000E+01 volume  0.69883E+03 ppm1      8.871 ppm2      8.719
ASSI [ 1031]
   (( segid "BrD " and resid 76   and name HN  ))
   (( segid "BrD " and resid 76   and name HA  ))
     2.500      1.600      1.600 peak  1031 weight  0.11000E+01 volume  0.86678E+03 ppm1      8.611 ppm2      4.688
ASSI [ 1041]
   (( segid "BrD " and resid 76   and name HN  ))
   ( segid "BrD " and resid 76   and name HB% )
     2.200      1.200      1.200 peak  1041 weight  0.11000E+01 volume  0.16592E+04 ppm1      8.612 ppm2      2.102
ASSI [ 1061]
   (( segid "BrD " and resid 77   and name HN  ))
   (( segid "BrD " and resid 77   and name HA  ))
     2.700      1.800      1.800 peak  1061 weight  0.11000E+01 volume  0.53554E+03 ppm1      7.996 ppm2      4.980
ASSI [ 1071]
   (( segid "BrD " and resid 77   and name HN  ))
   (( segid "BrD " and resid 77   and name HB1 ))
     2.100      1.100      1.100 peak  1071 weight  0.11000E+01 volume  0.22098E+04 ppm1      7.996 ppm2      3.337
ASSI [ 1091]
   (( segid "BrD " and resid 76   and name HN  ))
   (( segid "BrD " and resid 77   and name HN  ))
     2.600      1.700      1.700 peak  1091 weight  0.11000E+01 volume  0.57823E+03 ppm1      8.612 ppm2      7.983
ASSI [ 1111]
   (( segid "BrD " and resid 78   and name HN  ))
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   (( segid "BrD " and resid 75   and name HA  ))
      2.800     2.000     2.000 peak  1111 weight  0.11000E+01 volume  0.40919E+03 ppm1      9.106 ppm2      4.527
 ASSI { 1121}
   (( segid "BrD " and resid 75   and name HN  ))
   (( segid "BrD " and resid 75   and name HG1 ))
      2.600     1.700     1.700 peak  1121 weight  0.11000E+01 volume  0.66185E+03 ppm1      9.106 ppm2      3.549
 ASSI { 1131}
   (( segid "BrD " and resid 75   and name HN  ))
   (( segid "BrD " and resid 75   and name HG2 ))
      2.900     2.100     2.100 peak  1131 weight  0.11000E+01 volume  0.30957E+03 ppm1      9.106 ppm2      3.221
 ASSI { 1141}
   (( segid "BrD " and resid 75   and name HN  ))
   (( segid "BrD " and resid 75   and name HB1 ))
      3.100     2.400     2.400 peak  1141 weight  0.11000E+01 volume  0.19539E+03 ppm1      9.106 ppm2      2.919
 ASSI { 1151}
   (( segid "BrD " and resid 75   and name HN  ))
   (( segid "BrD " and resid 75   and name HB2 ))
      2.500     1.600     1.600 peak  1151 weight  0.11000E+01 volume  0.72202E+03 ppm1      9.106 ppm2      2.816
 ASSI { 1171}
   (( segid "BrD " and resid 76   and name HN  ))
   (( segid "BrD " and resid 75   and name HN  ))
      2.700     1.800     1.800 peak  1171 weight  0.11000E+01 volume  0.51792E+03 ppm1      8.613 ppm2      9.085
 ASSI { 1181}
   (( segid "BrD " and resid 74   and name HN  ))
   (  segid "BrD " and resid 74   and name HD% )
      3.000     2.200     2.200 peak  1181 weight  0.11000E+01 volume  0.24258E+03 ppm1      7.536 ppm2      7.004
 ASSI { 1191}
   (( segid "BrD " and resid 74   and name HN  ))
   (( segid "BrD " and resid 74   and name HA  ))
      3.000     2.200     2.200 peak  1191 weight  0.11000E+01 volume  0.27313E+03 ppm1      7.536 ppm2      4.368
 ASSI { 1201}
   (( segid "BrD " and resid 74   and name HN  ))
   (( segid "BrD " and resid 74   and name HB1 ))
      2.800     2.000     2.000 peak  1201 weight  0.11000E+01 volume  0.42552E+03 ppm1      7.535 ppm2      3.552
 ASSI { 1211}
   (( segid "BrD " and resid 74   and name HN  ))
   (( segid "BrD " and resid 74   and name HB2 ))
      2.700     1.800     1.800 peak  1211 weight  0.11000E+01 volume  0.47386E+03 ppm1      7.536 ppm2      2.983
 ASSI { 1231}
   (( segid "BrD " and resid 75   and name HN  ))
   (( segid "BrD " and resid 74   and name HN  ))
      2.800     2.000     2.000 peak  1231 weight  0.11000E+01 volume  0.42446E+03 ppm1      9.105 ppm2      7.535
 ASSI { 1241}
   (( segid "BrD " and resid 70   and name HN  ))
   (( segid "BrD " and resid 70   and name HA  ))
      2.500     1.600     1.600 peak  1241 weight  0.11000E+01 volume  0.78559E+03 ppm1      8.040 ppm2      5.348
 ASSI { 1251}
   (( segid "BrD " and resid 70   and name HN  ))
   (( segid "BrD " and resid 70   and name HB2 ))
      2.900     2.100     2.100 peak  1251 weight  0.11000E+01 volume  0.29096E+03 ppm1      8.039 ppm2      4.357
 ASSI { 1261}
   (( segid "BrD " and resid 69   and name HN  ))
   (( segid "BrD " and resid 69   and name HA  ))
      2.800     2.000     2.000 peak  1261 weight  0.11000E+01 volume  0.43807E+03 ppm1      8.306 ppm2      4.690
 ASSI { 1271}
   (( segid "BrD " and resid 69   and name HN  ))
   (( segid "BrD " and resid 69   and name HB  ))
      3.300     2.700     2.200 peak  1271 weight  0.11000E+01 volume  0.13733E+03 ppm1      8.306 ppm2      2.921
 ASSI { 1281}
   (( segid "BrD " and resid 69   and name HN  ))
   (  segid "BrD " and resid 69   and name HG1% )
      2.800     2.000     2.000 peak  1281 weight  0.11000E+01 volume  0.40608E+03 ppm1      8.306 ppm2      1.549
 ASSI { 1291}
   (( segid "BrD " and resid 69   and name HN  ))
   (  segid "BrD " and resid 69   and name HG2% )
      3.000     2.200     2.200 peak  1291 weight  0.11000E+01 volume  0.24335E+03 ppm1      8.306 ppm2      1.430
 ASSI { 1301}
   (( segid "BrD " and resid 69   and name HN  ))
   (( segid "BrD " and resid 70   and name HN  ))
      2.800     2.000     2.000 peak  1301 weight  0.11000E+01 volume  0.40402E+03 ppm1      8.306 ppm2      6.022
 ASSI { 1321}
   (( segid "BrD " and resid 68   and name HN  ))
   (  segid "BrD " and resid 68   and name HD% )
      2.900     2.100     2.100 peak  1321 weight  0.11000E+01 volume  0.34716E+03 ppm1      8.626 ppm2      7.778
 ASSI { 1331}
   (( segid "BrD " and resid 68   and name HN  ))
   (( segid "BrD " and resid 68   and name HA  ))
      3.200     2.600     2.300 peak  1331 weight  0.11000E+01 volume  0.16288E+03 ppm1      8.626 ppm2      5.142
 ASSI { 1341}
   (( segid "BrD " and resid 68   and name HN  ))
   (( segid "BrD " and resid 68   and name HB1 ))
      3.000     2.200     2.200 peak  1341 weight  0.11000E+01 volume  0.26781E+03 ppm1      8.625 ppm2      3.669
 ASSI { 1351}
   (( segid "BrD " and resid 68   and name HN  ))
   (( segid "BrD " and resid 68   and name HB2 ))
      2.700     1.800     1.800 peak  1351 weight  0.11000E+01 volume  0.52551E+03 ppm1      8.627 ppm2      3.516
 ASSI { 1361}
   (( segid "BrD " and resid 68   and name HN  ))
   (( segid "BrD " and resid 69   and name HN  ))
      3.500     3.100     2.000 peak  1361 weight  0.11000E+01 volume  0.11066E+03 ppm1      8.622 ppm2      8.304
 ASSI { 1381}
   (( segid "BrD " and resid 67   and name HN  ))
   (  segid "BrD " and resid 67   and name HD% )
      3.100     2.400     2.400 peak  1381 weight  0.11000E+01 volume  0.20078E+03 ppm1      8.832 ppm2      6.888
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 ASSI { 1391}
   (( segid "BrD " and resid 67   and name HN  ))
   (( segid "BrD " and resid 67   and name HA  ))
      2.800     2.000     2.000 peak  1391 weight  0.11000E+01 volume  0.36081E+03 ppm1      8.832 ppm2      4.671
 ASSI { 1401}
   (( segid "BrD " and resid 67   and name HN  ))
   (( segid "BrD " and resid 67   and name HB1 ))
      2.900     2.100     2.100 peak  1401 weight  0.11000E+01 volume  0.31437E+03 ppm1      8.832 ppm2      3.549
 ASSI { 1411}
   (( segid "BrD " and resid 67   and name HN  ))
   (( segid "BrD " and resid 67   and name HB2 ))
      2.400     1.400     1.400 peak  1411 weight  0.11000E+01 volume  0.92322E+03 ppm1      8.833 ppm2      2.661
 ASSI { 1431}
   (( segid "BrD " and resid 66   and name HN  ))
   (( segid "BrD " and resid 67   and name HN  ))
      2.500     1.600     1.600 peak  1431 weight  0.11000E+01 volume  0.76621E+03 ppm1      8.622 ppm2      8.829
 ASSI { 1441}
   (( segid "BrD " and resid 66   and name HN  ))
   (  segid "BrD " and resid 67   and name HD% )
      3.200     2.600     2.300 peak  1441 weight  0.11000E+01 volume  0.16656E+03 ppm1      8.626 ppm2      6.892
 ASSI { 1451}
   (( segid "BrD " and resid 66   and name HN  ))
   (( segid "BrD " and resid 66   and name HA  ))
      2.200     1.200     1.200 peak  1451 weight  0.11000E+01 volume  0.17604E+04 ppm1      8.763 ppm2      5.001
 ASSI { 1461}
   (( segid "BrD " and resid 65   and name HN  ))
   (( segid "BrD " and resid 65   and name HA  ))
      2.500     1.600     1.600 peak  1461 weight  0.11000E+01 volume  0.81596E+03 ppm1      8.564 ppm2      5.375
 ASSI { 1471}
   (( segid "BrD " and resid 65   and name HN  ))
   (( segid "BrD " and resid 65   and name HB1 ))
      2.600     1.700     1.700 peak  1471 weight  0.11000E+01 volume  0.66517E+03 ppm1      8.566 ppm2      3.627
 ASSI { 1481}
   (( segid "BrD " and resid 65   and name HN  ))
   (( segid "BrD " and resid 65   and name HB2 ))
      2.400     1.400     1.400 peak  1481 weight  0.11000E+01 volume  0.98393E+03 ppm1      8.564 ppm2      3.382
 ASSI { 1491}
   (( segid "BrD " and resid 65   and name HN  ))
   (( segid "BrD " and resid 64   and name HB1 ))
      2.400     1.400     1.400 peak  1491 weight  0.11000E+01 volume  0.10161E+04 ppm1      8.565 ppm2      2.659
 ASSI { 1501}
   (( segid "BrD " and resid 65   and name HN  ))
   (( segid "BrD " and resid 66   and name HN  ))
      2.300     1.300     1.300 peak  1501 weight  0.11000E+01 volume  0.13482E+04 ppm1      8.565 ppm2      8.765
 ASSI { 1521}
   (( segid "BrD " and resid 20   and name HN  ))
   (( segid "BrD " and resid 16   and name HA  ))
      2.700     1.800     1.800 peak  1521 weight  0.11000E+01 volume  0.44067E+03 ppm1      8.146 ppm2      4.527
 ASSI { 1531}
   (( segid "BrD " and resid 20   and name HN  ))
   (( segid "BrD " and resid 20   and name HA  ))
      2.500     1.600     1.600 peak  1531 weight  0.11000E+01 volume  0.84286E+03 ppm1      8.146 ppm2      4.895
 ASSI { 1541}
   (( segid "BrD " and resid 20   and name HN  ))
   (( segid "BrD " and resid 20   and name HB1 ))
      2.300     1.300     1.300 peak  1541 weight  0.11000E+01 volume  0.13472E+04 ppm1      8.147 ppm2      4.669
 ASSI { 1561}
   (( segid "BrD " and resid 21   and name HN  ))
   (( segid "BrD " and resid 21   and name HA  ))
      2.900     2.100     2.100 peak  1561 weight  0.11000E+01 volume  0.31054E+03 ppm1      8.546 ppm2      4.367
 ASSI { 1571}
   (( segid "BrD " and resid 101  and name HN  ))
   (( segid "BrD " and resid 101  and name HB  ))
      2.700     1.800     1.800 peak  1571 weight  0.11000E+01 volume  0.51528E+03 ppm1      8.514 ppm2      2.538
 ASSI { 1581}
   (( segid "BrD " and resid 22   and name HN  ))
   (( segid "BrD " and resid 22   and name HA  ))
      2.700     1.800     1.800 peak  1581 weight  0.11000E+01 volume  0.45405E+03 ppm1      9.456 ppm2      4.712
 ASSI { 1591}
   (( segid "BrD " and resid 23   and name HN  ))
   (( segid "BrD " and resid 21   and name HB  ))
      3.300     2.700     2.200 peak  1591 weight  0.11000E+01 volume  0.13959E+03 ppm1      9.122 ppm2      2.486
 ASSI { 1601}
   (( segid "BrD " and resid 23   and name HN  ))
   (( segid "BrD " and resid 23   and name HA  ))
      2.600     1.700     1.700 peak  1601 weight  0.11000E+01 volume  0.61098E+03 ppm1      9.118 ppm2      4.645
 ASSI { 1611}
   (( segid "BrD " and resid 23   and name HN  ))
   (( segid "BrD " and resid 23   and name HG1 ))
      3.400     2.900     2.100 peak  1611 weight  0.11000E+01 volume  0.11565E+03 ppm1      9.119 ppm2      3.143
 ASSI { 1621}
   (( segid "BrD " and resid 23   and name HN  ))
   (( segid "BrD " and resid 23   and name HB1 ))
      2.900     2.100     2.100 peak  1621 weight  0.11000E+01 volume  0.34650E+03 ppm1      9.118 ppm2      2.939
 ASSI { 1641}
   (( segid "BrD " and resid 22   and name HN  ))
   (( segid "BrD " and resid 23   and name HN  ))
      2.600     1.700     1.700 peak  1641 weight  0.11000E+01 volume  0.57061E+03 ppm1      9.456 ppm2      9.123
 ASSI { 1651}
   (( segid "BrD " and resid 15   and name HN  ))
   (  segid "BrD " and resid 15   and name HD% )
      3.100     2.400     2.400 peak  1651 weight  0.11000E+01 volume  0.20888E+03 ppm1      8.598 ppm2      7.663
 ASSI { 1661}
   (( segid "BrD " and resid 24   and name HN  ))
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   (( segid "BrD " and resid 24   and name HA  ))
      2.800     2.000     2.000 peak  1661 weight  0.11000E+01 volume  0.43492E+03 ppm1      8.661 ppm2      4.775
ASSI { 1671}
   (( segid "BrD " and resid 24   and name HN  ))
   (( segid "BrD " and resid 24   and name HG1 ))
      2.800     2.000     2.000 peak  1671 weight  0.11000E+01 volume  0.42365E+03 ppm1      8.660 ppm2      3.454
ASSI { 1681}
   (( segid "BrD " and resid 24   and name HN  ))
   (( segid "BrD " and resid 24   and name HB1 ))
      2.800     2.000     2.000 peak  1681 weight  0.11000E+01 volume  0.37096E+03 ppm1      8.654 ppm2      3.089
ASSI { 1691}
   (( segid "BrD " and resid 24   and name HN  ))
   (( segid "BrD " and resid 23   and name HN  ))
      2.300     1.300     1.300 peak  1691 weight  0.11000E+01 volume  0.12196E+04 ppm1      8.659 ppm2      9.112
ASSI { 1711}
   (( segid "BrD " and resid 25   and name HN  ))
   (( segid "BrD " and resid 27   and name HN  ))
      3.600     3.200     1.900 peak  1711 weight  0.11000E+01 volume  0.81722E+02 ppm1      9.134 ppm2      8.155
ASSI { 1721}
   (( segid "BrD " and resid 25   and name HN  ))
   (( segid "BrD " and resid 25   and name HA  ))
      3.200     2.600     2.300 peak  1721 weight  0.11000E+01 volume  0.16529E+03 ppm1      9.134 ppm2      4.443
ASSI { 1731}
   (( segid "BrD " and resid 25   and name HN  ))
   (( segid "BrD " and resid 25   and name HB  ))
      2.800     2.000     2.000 peak  1731 weight  0.11000E+01 volume  0.35564E+03 ppm1      9.132 ppm2      2.984
ASSI { 1741}
   (( segid "BrD " and resid 25   and name HN  ))
   (  segid "BrD " and resid 25   and name HG1%)
      2.600     1.700     1.700 peak  1741 weight  0.11000E+01 volume  0.61322E+03 ppm1      9.133 ppm2      1.799
ASSI { 1751}
   (( segid "BrD " and resid 25   and name HN  ))
   (  segid "BrD " and resid 25   and name HG2%)
      2.800     2.000     2.000 peak  1751 weight  0.11000E+01 volume  0.35918E+03 ppm1      9.133 ppm2      1.627
ASSI { 1771}
   (( segid "BrD " and resid 24   and name HN  ))
   (( segid "BrD " and resid 25   and name HN  ))
      2.400     1.400     1.400 peak  1771 weight  0.11000E+01 volume  0.91823E+03 ppm1      8.661 ppm2      9.133
ASSI { 1791}
   (( segid "BrD " and resid 26   and name HN  ))
   (( segid "BrD " and resid 26   and name HA  ))
      3.000     2.200     2.200 peak  1791 weight  0.11000E+01 volume  0.24501E+03 ppm1      9.196 ppm2      4.488
ASSI { 1801}
   (( segid "BrD " and resid 27   and name HN  ))
   (( segid "BrD " and resid 26   and name HB1 ))
      2.700     1.800     1.800 peak  1801 weight  0.11000E+01 volume  0.50197E+03 ppm1      8.169 ppm2      2.480
ASSI { 1811}
   (( segid "BrD " and resid 27   and name HN  ))
   (( segid "BrD " and resid 27   and name HA  ))
      2.700     1.800     1.800 peak  1811 weight  0.11000E+01 volume  0.49453E+03 ppm1      8.170 ppm2      5.055
ASSI { 1821}
   (( segid "BrD " and resid 27   and name HN  ))
   (( segid "BrD " and resid 27   and name HB1 ))
      2.500     1.600     1.600 peak  1821 weight  0.11000E+01 volume  0.78563E+03 ppm1      8.170 ppm2      4.611
ASSI { 1831}
   (( segid "BrD " and resid 27   and name HN  ))
   (( segid "BrD " and resid 26   and name HN  ))
      2.600     1.700     1.700 peak  1831 weight  0.11000E+01 volume  0.56681E+03 ppm1      8.169 ppm2      9.179
ASSI { 1851}
   (( segid "BrD " and resid 19   and name HN  ))
   (( segid "BrD " and resid 15   and name HA  ))
      3.100     2.400     2.400 peak  1851 weight  0.11000E+01 volume  0.20055E+03 ppm1      9.187 ppm2      4.645
ASSI { 1861}
   (( segid "BrD " and resid 19   and name HN  ))
   (( segid "BrD " and resid 19   and name HA  ))
      2.800     2.000     2.000 peak  1861 weight  0.11000E+01 volume  0.37223E+03 ppm1      9.189 ppm2      4.285
ASSI { 1881}
   (( segid "BrD " and resid 20   and name HN  ))
   (( segid "BrD " and resid 19   and name HN  ))
      2.800     2.000     2.000 peak  1881 weight  0.11000E+01 volume  0.39357E+03 ppm1      8.146 ppm2      9.170
ASSI { 1901}
   (( segid "BrD " and resid 83   and name HN  ))
   (( segid "BrD " and resid 83   and name HA  ))
      2.800     2.000     2.000 peak  1901 weight  0.11000E+01 volume  0.35792E+03 ppm1      9.658 ppm2      4.447
ASSI { 1911}
   (( segid "BrD " and resid 83   and name HN  ))
   (( segid "BrD " and resid 83   and name HB  ))
      2.700     1.800     1.800 peak  1911 weight  0.11000E+01 volume  0.45140E+03 ppm1      9.659 ppm2      4.817
ASSI { 1921}
   (( segid "BrD " and resid 83   and name HN  ))
   (  segid "BrD " and resid 83   and name HG2%)
      3.000     2.200     2.200 peak  1921 weight  0.11000E+01 volume  0.28097E+03 ppm1      9.659 ppm2      1.910
ASSI { 1931}
   (( segid "BrD " and resid 84   and name HN  ))
   (( segid "BrD " and resid 84   and name HA  ))
      2.800     2.000     2.000 peak  1931 weight  0.11000E+01 volume  0.37490E+03 ppm1      9.464 ppm2      4.901
ASSI { 1941}
   (( segid "BrD " and resid 84   and name HN  ))
   (( segid "BrD " and resid 84   and name HB1 ))
      2.800     2.000     2.000 peak  1941 weight  0.11000E+01 volume  0.42690E+03 ppm1      9.463 ppm2      3.592
ASSI { 1951}
   (( segid "BrD " and resid 84   and name HN  ))
   (( segid "BrD " and resid 84   and name HB2 ))
      3.000     2.200     2.200 peak  1951 weight  0.11000E+01 volume  0.26963E+03 ppm1      9.463 ppm2      3.368
ASSI { 1971}
   (( segid "BrD " and resid 83   and name HN  ))
   (( segid "BrD " and resid 84   and name HN  ))
      2.600     1.700     1.700 peak  1971 weight  0.11000E+01 volume  0.61276E+03 ppm1      9.658 ppm2      9.450
ASSI { 1981}
   (( segid "BrD " and resid 85   and name HN  ))
   (( segid "BrD " and resid 85   and name HA  ))
      2.900     2.100     2.100 peak  1981 weight  0.11000E+01 volume  0.32851E+03 ppm1      7.516 ppm2      5.014
ASSI { 1991}
   (( segid "BrD " and resid 85   and name HN  ))
   (( segid "BrD " and resid 85   and name HB1 ))
      2.800     2.000     2.000 peak  1991 weight  0.11000E+01 volume  0.39507E+03 ppm1      7.516 ppm2      3.919
ASSI { 2011}
   (( segid "BrD " and resid 84   and name HN  ))
   (( segid "BrD " and resid 85   and name HN  ))
      2.800     2.000     2.000 peak  2011 weight  0.11000E+01 volume  0.37475E+03 ppm1      9.464 ppm2      7.497
ASSI { 2021}
   (( segid "BrD " and resid 86   and name HN  ))
   (( segid "BrD " and resid 85   and name HB1 ))
      3.200     2.600     2.300 peak  2021 weight  0.11000E+01 volume  0.17051E+03 ppm1      8.423 ppm2      3.911
ASSI { 2031}
   (( segid "BrD " and resid 86   and name HN  ))
   (( segid "BrD " and resid 86   and name HA  ))
      2.800     2.000     2.000 peak  2031 weight  0.11000E+01 volume  0.42952E+03 ppm1      8.423 ppm2      4.809
ASSI { 2051}
   (( segid "BrD " and resid 85   and name HN  ))
   (( segid "BrD " and resid 86   and name HN  ))
      2.800     2.000     2.000 peak  2051 weight  0.11000E+01 volume  0.39765E+03 ppm1      7.516 ppm2      8.406
ASSI { 2061}
   (( segid "BrD " and resid 87   and name HN  ))
   (( segid "BrD " and resid 86   and name HB1 ))
      3.400     2.900     2.100 peak  2061 weight  0.11000E+01 volume  0.11283E+03 ppm1      8.570 ppm2      2.350
ASSI { 2071}
   (( segid "BrD " and resid 87   and name HN  ))
   (( segid "BrD " and resid 87   and name HA  ))
      2.600     1.700     1.700 peak  2071 weight  0.11000E+01 volume  0.62404E+03 ppm1      8.572 ppm2      4.889
ASSI { 2081}
   (( segid "BrD " and resid 87   and name HN  ))
   (( segid "BrD " and resid 87   and name HG1 ))
      3.000     2.200     2.200 peak  2081 weight  0.11000E+01 volume  0.28244E+03 ppm1      8.572 ppm2      3.014
ASSI { 2091}
   (( segid "BrD " and resid 87   and name HN  ))
   (( segid "BrD " and resid 87   and name HG2 ))
      3.000     2.200     2.200 peak  2091 weight  0.11000E+01 volume  0.28579E+03 ppm1      8.570 ppm2      2.610
ASSI { 2101}
   (( segid "BrD " and resid 87   and name HN  ))
   (( segid "BrD " and resid 87   and name HB2 ))
      2.700     1.800     1.800 peak  2101 weight  0.11000E+01 volume  0.46735E+03 ppm1      8.571 ppm2      2.607
ASSI { 2111}
   (( segid "BrD " and resid 88   and name HN  ))
   (  segid "BrD " and resid 88   and name HD% )
      3.300     2.700     2.200 peak  2111 weight  0.11000E+01 volume  0.15320E+03 ppm1      8.355 ppm2      7.595
ASSI { 2121}
   (( segid "BrD " and resid 88   and name HN  ))
   (( segid "BrD " and resid 88   and name HA  ))
      3.100     2.400     2.400 peak  2121 weight  0.11000E+01 volume  0.22276E+03 ppm1      8.356 ppm2      4.976
ASSI { 2131}
   (( segid "BrD " and resid 88   and name HN  ))
   (( segid "BrD " and resid 88   and name HB1 ))
      2.500     1.600     1.600 peak  2131 weight  0.11000E+01 volume  0.72297E+03 ppm1      8.354 ppm2      3.536
ASSI { 2151}
   (( segid "BrD " and resid 89   and name HN  ))
   (( segid "BrD " and resid 89   and name HA  ))
      3.000     2.200     2.200 peak  2151 weight  0.11000E+01 volume  0.26347E+03 ppm1      8.858 ppm2      5.631
ASSI { 2161}
   (( segid "BrD " and resid 89   and name HN  ))
   (( segid "BrD " and resid 89   and name HB1 ))
      3.000     2.200     2.200 peak  2161 weight  0.11000E+01 volume  0.26996E+03 ppm1      8.858 ppm2      3.671
ASSI { 2171}
   (( segid "BrD " and resid 89   and name HN  ))
   (( segid "BrD " and resid 89   and name HB2 ))
      2.400     1.400     1.400 peak  2171 weight  0.11000E+01 volume  0.10141E+04 ppm1      8.858 ppm2      3.508
ASSI { 2191}
   (( segid "BrD " and resid 88   and name HN  ))
   (( segid "BrD " and resid 89   and name HN  ))
      2.600     1.700     1.700 peak  2191 weight  0.11000E+01 volume  0.62688E+03 ppm1      8.355 ppm2      8.848
ASSI { 2201}
   (( segid "BrD " and resid 46   and name HN  ))
   (( segid "BrD " and resid 47   and name HN  ))
      2.800     2.000     2.000 peak  2201 weight  0.11000E+01 volume  0.38079E+03 ppm1      8.562 ppm2      8.836
ASSI { 2211}
   (( segid "BrD " and resid 46   and name HN  ))
   (( segid "BrD " and resid 46   and name HA  ))
      2.700     1.800     1.800 peak  2211 weight  0.11000E+01 volume  0.49246E+03 ppm1      8.562 ppm2      4.125
ASSI { 2221}
   (( segid "BrD " and resid 46   and name HN  ))
   (( segid "BrD " and resid 46   and name HB1 ))
      2.500     1.600     1.600 peak  2221 weight  0.11000E+01 volume  0.82312E+03 ppm1      8.561 ppm2      3.293
ASSI { 2231}
   (( segid "BrD " and resid 46   and name HN  ))
   (( segid "BrD " and resid 46   and name HB2 ))
      2.500     1.600     1.600 peak  2231 weight  0.11000E+01 volume  0.72605E+03 ppm1      8.842 ppm2      3.098
ASSI { 2241}
   (( segid "BrD " and resid 47   and name HN  ))
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   ( segid "BrD " and resid 47   and name HE1 )
     3.700     3.400     1.800 peak  2241 weight  0.11000E+01 volume  0.71965E+02 ppm1      8.832 ppm2      7.253
ASSI { 2251}
   (( segid "BrD " and resid 47   and name HN  ))
   (( segid "BrD " and resid 47   and name HA  ))
     2.900     2.100     2.100 peak  2251 weight  0.11000E+01 volume  0.34426E+03 ppm1      8.831 ppm2      4.708
ASSI { 2261}
   (( segid "BrD " and resid 47   and name HN  ))
   (( segid "BrD " and resid 47   and name HB1 ))
     2.800     2.000     2.000 peak  2261 weight  0.11000E+01 volume  0.37083E+03 ppm1      8.833 ppm2      3.807
ASSI { 2271}
   (( segid "BrD " and resid 47   and name HN  ))
   (( segid "BrD " and resid 47   and name HB2 ))
     2.900     2.100     2.100 peak  2271 weight  0.11000E+01 volume  0.34763E+03 ppm1      8.832 ppm2      3.391
ASSI { 2281}
   (( segid "BrD " and resid 48   and name HN  ))
   (( segid "BrD " and resid 48   and name HA  ))
     2.800     2.000     2.000 peak  2281 weight  0.11000E+01 volume  0.37621E+03 ppm1      8.307 ppm2      4.615
ASSI { 2291}
   (( segid "BrD " and resid 48   and name HN  ))
   (( segid "BrD " and resid 48   and name HG2 ))
     3.300     2.700     2.200 peak  2291 weight  0.11000E+01 volume  0.14081E+03 ppm1      8.308 ppm2      2.857
ASSI { 2301}
   (( segid "BrD " and resid 48   and name HN  ))
   (( segid "BrD " and resid 48   and name HB1 ))
     2.400     1.400     1.400 peak  2301 weight  0.11000E+01 volume  0.11018E+04 ppm1      8.308 ppm2      2.698
ASSI { 2311}
   (( segid "BrD " and resid 47   and name HN  ))
   (( segid "BrD " and resid 48   and name HN  ))
     2.700     1.800     1.800 peak  2311 weight  0.11000E+01 volume  0.47004E+03 ppm1      8.832 ppm2      8.310
ASSI { 2341}
   (( segid "BrD " and resid 49   and name HN  ))
   (( segid "BrD " and resid 49   and name HA  ))
     2.600     1.700     1.700 peak  2341 weight  0.11000E+01 volume  0.63035E+03 ppm1      7.762 ppm2      4.690
ASSI { 2351}
   (( segid "BrD " and resid 49   and name HN  ))
   (( segid "BrD " and resid 49   and name HB  ))
     3.100     2.400     2.400 peak  2351 weight  0.11000E+01 volume  0.22961E+03 ppm1      7.762 ppm2      2.611
ASSI { 2361}
   (( segid "BrD " and resid 49   and name HN  ))
   ( segid "BrD " and resid 49   and name HG2%)
     3.300     2.700     2.200 peak  2361 weight  0.11000E+01 volume  0.15115E+03 ppm1      7.762 ppm2      1.586
ASSI { 2381}
   (( segid "BrD " and resid 48   and name HN  ))
   (( segid "BrD " and resid 49   and name HN  ))
     2.400     1.400     1.400 peak  2381 weight  0.11000E+01 volume  0.95252E+03 ppm1      8.308 ppm2      7.742
ASSI { 2391}
   (( segid "BrD " and resid 50   and name HN  ))
   (( segid "BrD " and resid 51   and name HN  ))
     2.600     1.700     1.700 peak  2391 weight  0.11000E+01 volume  0.55801E+03 ppm1      8.559 ppm2      8.318
ASSI { 2401}
   (( segid "BrD " and resid 50   and name HN  ))
   (( segid "BrD " and resid 50   and name HA  ))
     2.700     1.800     1.800 peak  2401 weight  0.11000E+01 volume  0.45800E+03 ppm1      8.564 ppm2      4.525
ASSI { 2421}
   (( segid "BrD " and resid 49   and name HN  ))
   (( segid "BrD " and resid 50   and name HN  ))
     2.400     1.400     1.400 peak  2421 weight  0.11000E+01 volume  0.91502E+03 ppm1      7.762 ppm2      8.554
ASSI { 2431}
   (( segid "BrD " and resid 115  and name HN  ))
   (( segid "BrD " and resid 114  and name HA2 ))
     3.100     2.400     2.400 peak  2431 weight  0.11000E+01 volume  0.20145E+03 ppm1      8.355 ppm2      4.542
ASSI { 2441}
   (( segid "BrD " and resid 115  and name HN  ))
   (( segid "BrD " and resid 115  and name HA  ))
     2.800     2.000     2.000 peak  2441 weight  0.11000E+01 volume  0.38387E+03 ppm1      8.355 ppm2      4.822
ASSI { 2451}
   (( segid "BrD " and resid 116  and name HN  ))
   (( segid "BrD " and resid 115  and name HB1 ))
     2.700     1.800     1.800 peak  2451 weight  0.11000E+01 volume  0.51528E+03 ppm1      8.086 ppm2      2.169
ASSI { 2461}
   (( segid "BrD " and resid 116  and name HN  ))
   (( segid "BrD " and resid 116  and name HA  ))
     2.500     1.600     1.600 peak  2461 weight  0.11000E+01 volume  0.81456E+03 ppm1      8.087 ppm2      4.828
ASSI { 2471}
   (( segid "BrD " and resid 116  and name HN  ))
   (( segid "BrD " and resid 116  and name HB  ))
     2.600     1.700     1.700 peak  2471 weight  0.11000E+01 volume  0.58085E+03 ppm1      8.086 ppm2      2.419
ASSI { 2481}
   (( segid "BrD " and resid 117  and name HN  ))
   (( segid "BrD " and resid 117  and name HA  ))
     3.300     2.700     2.200 peak  2481 weight  0.11000E+01 volume  0.15334E+03 ppm1      8.880 ppm2      5.171
ASSI { 2491}
   (( segid "BrD " and resid 117  and name HN  ))
   (( segid "BrD " and resid 117  and name HB1 ))
     3.300     2.700     2.200 peak  2491 weight  0.11000E+01 volume  0.14660E+03 ppm1      8.879 ppm2      3.300
ASSI { 2501}
   (( segid "BrD " and resid 117  and name HN  ))
   (( segid "BrD " and resid 117  and name HB2 ))
     2.800     2.000     2.000 peak  2501 weight  0.11000E+01 volume  0.41931E+03 ppm1      8.879 ppm2      3.147
ASSI { 2511}
   (( segid "BrD " and resid 51   and name HN  ))
   (( segid "BrD " and resid 51   and name HA  ))
     2.300     1.300     1.300 peak  2511 weight  0.11000E+01 volume  0.13843E+04 ppm1      8.377 ppm2      4.475
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ASSI { 2521}
   (( segid "BrD " and resid 51   and name HN  ))
   (( segid "BrD " and resid 51   and name HG1 ))
     2.900     2.100     2.100 peak  2521 weight  0.11000E+01 volume  0.29957E+03 ppm1      8.375 ppm2      1.933
ASSI { 2531}
   (( segid "BrD " and resid 17   and name HN  ))
   (( segid "BrD " and resid 17   and name HB  ))
     3.000     2.200     2.200 peak  2531 weight  0.11000E+01 volume  0.26023E+03 ppm1      8.679 ppm2      4.860
ASSI { 2541}
   (( segid "BrD " and resid 17   and name HN  ))
   (( segid "BrD " and resid 17   and name HA  ))
     2.400     1.400     1.400 peak  2541 weight  0.11000E+01 volume  0.10062E+04 ppm1      8.678 ppm2      4.571
ASSI { 2551}
   (( segid "BrD " and resid 17   and name HN  ))
   ( segid "BrD " and resid 17   and name HG2%)
     3.100     2.400     2.400 peak  2551 weight  0.11000E+01 volume  0.20185E+03 ppm1      8.670 ppm2      1.745
ASSI { 2561}
   (( segid "BrD " and resid 101  and name HN  ))
   (( segid "BrD " and resid 100  and name HB2 ))
     2.800     2.000     2.000 peak  2561 weight  0.11000E+01 volume  0.38883E+03 ppm1      8.513 ppm2      3.441
ASSI { 2571}
   (( segid "BrD " and resid 101  and name HN  ))
   (( segid "BrD " and resid 101  and name HA  ))
     2.800     2.000     2.000 peak  2571 weight  0.11000E+01 volume  0.37743E+03 ppm1      8.513 ppm2      4.264
ASSI { 2591}
   (( segid "BrD " and resid 100  and name HN  ))
   (( segid "BrD " and resid 101  and name HN  ))
     2.600     1.700     1.700 peak  2591 weight  0.11000E+01 volume  0.62929E+03 ppm1      8.669 ppm2      8.521
ASSI { 2601}
   (( segid "BrD " and resid 102  and name HN  ))
   (( segid "BrD " and resid 102  and name HA  ))
     2.900     2.100     2.100 peak  2601 weight  0.11000E+01 volume  0.34745E+03 ppm1      9.156 ppm2      4.280
ASSI { 2611}
   (( segid "BrD " and resid 102  and name HN  ))
   (( segid "BrD " and resid 101  and name HN  ))
     2.700     1.800     1.800 peak  2611 weight  0.11000E+01 volume  0.52631E+03 ppm1      9.156 ppm2      8.513
ASSI { 2641}
   (( segid "BrD " and resid 103  and name HN  ))
   (( segid "BrD " and resid 103  and name HA  ))
     2.800     2.000     2.000 peak  2641 weight  0.11000E+01 volume  0.41836E+03 ppm1      8.695 ppm2      3.800
ASSI { 2651}
   (( segid "BrD " and resid 103  and name HN  ))
   (( segid "BrD " and resid 103  and name HB2 ))
     2.800     2.000     2.000 peak  2651 weight  0.11000E+01 volume  0.35593E+03 ppm1      8.696 ppm2      1.928
ASSI { 2661}
   (( segid "BrD " and resid 103  and name HN  ))
   (( segid "BrD " and resid 103  and name HB1 ))
     2.500     1.600     1.600 peak  2661 weight  0.11000E+01 volume  0.72768E+03 ppm1      8.695 ppm2      2.353
ASSI { 2671}
   (( segid "BrD " and resid 103  and name HN  ))
   (( segid "BrD " and resid 103  and name HG2 ))
     3.200     2.600     2.300 peak  2671 weight  0.11000E+01 volume  0.18331E+03 ppm1      8.695 ppm2      2.529
ASSI { 2681}
   (( segid "BrD " and resid 103  and name HN  ))
   (( segid "BrD " and resid 102  and name HN  ))
     2.600     1.700     1.700 peak  2681 weight  0.11000E+01 volume  0.68597E+03 ppm1      8.694 ppm2      9.157
ASSI { 2711}
   (( segid "BrD " and resid 104  and name HN  ))
   (( segid "BrD " and resid 104  and name HA  ))
     2.600     1.700     1.700 peak  2711 weight  0.11000E+01 volume  0.66065E+03 ppm1      7.763 ppm2      4.690
ASSI { 2731}
   (( segid "BrD " and resid 104  and name HN  ))
   (( segid "BrD " and resid 103  and name HN  ))
     2.800     2.000     2.000 peak  2731 weight  0.11000E+01 volume  0.40496E+03 ppm1      7.763 ppm2      8.680
ASSI { 2751}
   (( segid "BrD " and resid 104  and name HN  ))
   (( segid "BrD " and resid 105  and name HN  ))
     2.700     1.800     1.800 peak  2751 weight  0.11000E+01 volume  0.54532E+03 ppm1      7.763 ppm2      8.475
ASSI { 2771}
   (( segid "BrD " and resid 79   and name HN  ))
   ( segid "BrD " and resid 78   and name HD1%)
     3.900     3.800     1.600 peak  2771 weight  0.11000E+01 volume  0.50980E+02 ppm1      8.685 ppm2      0.788
ASSI { 2781}
   (( segid "BrD " and resid 81   and name HN  ))
   (( segid "BrD " and resid 81   and name HA  ))
     3.300     2.700     2.200 peak  2781 weight  0.11000E+01 volume  0.15663E+03 ppm1      7.640 ppm2      3.711
ASSI { 2791}
   (( segid "BrD " and resid 81   and name HN  ))
   (( segid "BrD " and resid 81   and name HB  ))
     2.500     1.600     1.600 peak  2791 weight  0.11000E+01 volume  0.72728E+03 ppm1      7.640 ppm2      2.037
ASSI { 2801}
   (( segid "BrD " and resid 81   and name HN  ))
   ( segid "BrD " and resid 81   and name HG1%)
     2.500     1.600     1.600 peak  2801 weight  0.11000E+01 volume  0.82553E+03 ppm1      7.640 ppm2      1.071
ASSI { 2811}
   (( segid "BrD " and resid 81   and name HN  ))
   ( segid "BrD " and resid 81   and name HG2%)
     3.100     2.400     2.400 peak  2811 weight  0.11000E+01 volume  0.22921E+03 ppm1      7.640 ppm2      0.751
ASSI { 2821}
   (( segid "BrD " and resid 82   and name HN  ))
   ( segid "BrD " and resid 82   and name HD% )
     3.000     3.200     2.200 peak  2821 weight  0.11000E+01 volume  0.28368E+03 ppm1      6.981 ppm2      7.286
ASSI { 2831}
   (( segid "BrD " and resid 82   and name HN  ))
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   (( segid "BrD " and resid 82   and name HA  ))
      2.800     2.000     2.000 peak  2831 weight  0.11000E+01 volume  0.42147E+03 ppm1     6.981 ppm2     4.738
ASSI { 2841}
   (( segid "BrD " and resid 82   and name HN  ))
   (( segid "BrD " and resid 82   and name HB1 ))
      3.000     2.200     2.200 peak  2841 weight  0.11000E+01 volume  0.27134E+03 ppm1     6.981 ppm2     3.706
ASSI { 2851}
   (( segid "BrD " and resid 82   and name HN  ))
   (( segid "BrD " and resid 82   and name HB2 ))
      2.600     1.700     1.700 peak  2851 weight  0.11000E+01 volume  0.58897E+03 ppm1     6.981 ppm2     3.556
ASSI { 2871}
   (( segid "BrD " and resid 81   and name HN  ))
   (( segid "BrD " and resid 82   and name HN  ))
      2.800     2.000     2.000 peak  2871 weight  0.11000E+01 volume  0.36428E+03 ppm1     7.640 ppm2     6.966
ASSI { 2891}
   (( segid "BrD " and resid 82   and name HN  ))
   (( segid "BrD " and resid 83   and name HN  ))
      2.800     2.000     2.000 peak  2891 weight  0.11000E+01 volume  0.41793E+03 ppm1     6.981 ppm2     9.658
ASSI { 2901}
   (( segid "BrD " and resid 79   and name HN  ))
   (  segid "BrD " and resid 78   and name HD2%)
      3.900     3.800     1.600 peak  2901 weight  0.11000E+01 volume  0.52951E+02 ppm1     8.684 ppm2     0.666
ASSI { 2911}
   (( segid "BrD " and resid 80   and name HN  ))
   (( segid "BrD " and resid 80   and name HA  ))
      2.500     1.600     1.600 peak  2911 weight  0.11000E+01 volume  0.82068E+03 ppm1     8.005 ppm2     4.678
ASSI { 2921}
   (( segid "BrD " and resid 80   and name HN  ))
   (( segid "BrD " and resid 81   and name HN  ))
      2.700     1.800     1.800 peak  2921 weight  0.11000E+01 volume  0.47132E+03 ppm1     8.006 ppm2     7.632
ASSI { 2941}
   (( segid "BrD " and resid 83   and name HN  ))
   (  segid "BrD " and resid 82   and name HD% )
      3.400     2.900     2.100 peak  2941 weight  0.11000E+01 volume  0.12712E+03 ppm1     9.658 ppm2     7.248
ASSI { 2951}
   (( segid "BrD " and resid 79   and name HN  ))
   (( segid "BrD " and resid 79   and name HA  ))
      2.600     1.700     1.700 peak  2951 weight  0.11000E+01 volume  0.57656E+03 ppm1     8.681 ppm2     4.406
ASSI { 2961}
   (( segid "BrD " and resid 79   and name HN  ))
   (( segid "BrD " and resid 79   and name HG1 ))
      2.900     2.100     2.100 peak  2961 weight  0.11000E+01 volume  0.30890E+03 ppm1     8.681 ppm2     3.055
ASSI { 2971}
   (( segid "BrD " and resid 79   and name HN  ))
   (( segid "BrD " and resid 79   and name HB2 ))
      2.500     1.600     1.600 peak  2971 weight  0.11000E+01 volume  0.78107E+03 ppm1     8.679 ppm2     2.684
ASSI { 2981}
   (( segid "BrD " and resid 80   and name HN  ))
   (( segid "BrD " and resid 79   and name HN  ))
      2.700     1.800     1.800 peak  2981 weight  0.11000E+01 volume  0.45960E+03 ppm1     8.006 ppm2     8.676
ASSI { 3001}
   (( segid "BrD " and resid 74   and name HN  ))
   (( segid "BrD " and resid 72   and name HA  ))
      3.500     3.100     2.000 peak  3001 weight  0.11000E+01 volume  0.98034E+02 ppm1     7.536 ppm2     4.666
ASSI { 3011}
   (( segid "BrD " and resid 73   and name HN  ))
   (( segid "BrD " and resid 73   and name HA  ))
      2.600     1.700     1.700 peak  3011 weight  0.11000E+01 volume  0.57896E+03 ppm1     8.045 ppm2     4.811
ASSI { 3021}
   (( segid "BrD " and resid 73   and name HN  ))
   (( segid "BrD " and resid 74   and name HN  ))
      2.800     2.000     2.000 peak  3021 weight  0.11000E+01 volume  0.42186E+03 ppm1     8.049 ppm2     7.542
ASSI { 3041}
   (( segid "BrD " and resid 64   and name HN  ))
   (( segid "BrD " and resid 63   and name HA  ))
      3.100     2.400     2.400 peak  3041 weight  0.11000E+01 volume  0.20596E+03 ppm1     8.584 ppm2     5.298
ASSI { 3051}
   (( segid "BrD " and resid 64   and name HN  ))
   (( segid "BrD " and resid 64   and name HA  ))
      2.600     1.700     1.700 peak  3051 weight  0.11000E+01 volume  0.63768E+03 ppm1     8.584 ppm2     4.940
ASSI { 3061}
   (( segid "BrD " and resid 63   and name HN  ))
   (( segid "BrD " and resid 63   and name HA  ))
      2.900     2.100     2.100 peak  3061 weight  0.11000E+01 volume  0.33289E+03 ppm1     9.473 ppm2     5.302
ASSI { 3071}
   (( segid "BrD " and resid 63   and name HN  ))
   (( segid "BrD " and resid 64   and name HN  ))
      2.600     1.700     1.700 peak  3071 weight  0.11000E+01 volume  0.68875E+03 ppm1     9.478 ppm2     8.565
ASSI { 3091}
   (( segid "BrD " and resid 38   and name HN  ))
   (( segid "BrD " and resid 38   and name HA  ))
      3.100     2.400     2.400 peak  3091 weight  0.11000E+01 volume  0.21794E+03 ppm1     8.732 ppm2     4.166
ASSI { 3101}
   (( segid "BrD " and resid 38   and name HN  ))
   (( segid "BrD " and resid 38   and name HB  ))
      2.500     1.600     1.600 peak  3101 weight  0.11000E+01 volume  0.76036E+03 ppm1     8.731 ppm2     1.767
ASSI { 3111}
   (( segid "BrD " and resid 38   and name HN  ))
   (  segid "BrD " and resid 38   and name HG1%)
      2.400     1.400     1.400 peak  3111 weight  0.11000E+01 volume  0.94284E+03 ppm1     8.733 ppm2     1.071
ASSI { 3121}
   (( segid "BrD " and resid 38   and name HN  ))
   (  segid "BrD " and resid 38   and name HG2%)
      4.000     4.000     1.500 peak  3121 weight  0.11000E+01 volume  0.47989E+02 ppm1     8.732 ppm2     0.784
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ASSI { 3131}
   (( segid "BrD " and resid 39   and name HN  ))
   (( segid "BrD " and resid 39   and name HA  ))
      3.600     3.200     1.900 peak  3131 weight  0.11000E+01 volume  0.90084E+02 ppm1     9.653 ppm2     4.977
ASSI { 3141}
   (( segid "BrD " and resid 58   and name HN  ))
   (( segid "BrD " and resid 58   and name HA  ))
      2.900     2.100     2.100 peak  3141 weight  0.11000E+01 volume  0.34424E+03 ppm1    10.051 ppm2     4.451
ASSI { 3151}
   (( segid "BrD " and resid 58   and name HN  ))
   (( segid "BrD " and resid 58   and name HB  ))
      2.900     2.100     2.100 peak  3151 weight  0.11000E+01 volume  0.30448E+03 ppm1    10.052 ppm2     4.686
ASSI { 3161}
   (( segid "BrD " and resid 58   and name HN  ))
   (  segid "BrD " and resid 58   and name HG2%)
      3.700     3.400     1.800 peak  3161 weight  0.11000E+01 volume  0.68430E+02 ppm1    10.051 ppm2     1.674
ASSI { 3171}
   (( segid "BrD " and resid 57   and name HN  ))
   (( segid "BrD " and resid 57   and name HA  ))
      2.700     1.800     1.800 peak  3171 weight  0.11000E+01 volume  0.45739E+03 ppm1     9.359 ppm2     4.809
ASSI { 3191}
   (( segid "BrD " and resid 58   and name HN  ))
   (( segid "BrD " and resid 57   and name HN  ))
      2.600     1.700     1.700 peak  3191 weight  0.11000E+01 volume  0.55403E+03 ppm1    10.051 ppm2     9.351
ASSI { 3201}
   (( segid "BrD " and resid 56   and name HN  ))
   (( segid "BrD " and resid 56   and name HA  ))
      3.100     2.400     2.400 peak  3201 weight  0.11000E+01 volume  0.22011E+03 ppm1     9.678 ppm2     4.622
ASSI { 3221}
   (( segid "BrD " and resid 57   and name HN  ))
   (( segid "BrD " and resid 56   and name HN  ))
      3.100     2.400     2.400 peak  3221 weight  0.11000E+01 volume  0.21874E+03 ppm1     9.359 ppm2     9.662
ASSI { 3231}
   (( segid "BrD " and resid 79   and name HN  ))
   (( segid "BrD " and resid 78   and name HN2 ))
      3.200     2.600     2.300 peak  3231 weight  0.11000E+01 volume  0.19421E+03 ppm1     8.680 ppm2     1.049
ASSI { 3241}
   (( segid "BrD " and resid 55   and name HN  ))
   (( segid "BrD " and resid 55   and name HA  ))
      2.600     1.700     1.700 peak  3241 weight  0.11000E+01 volume  0.57256E+03 ppm1     7.973 ppm2     5.343
ASSI { 3251}
   (( segid "BrD " and resid 55   and name HN  ))
   (( segid "BrD " and resid 55   and name HB1 ))
      3.200     2.600     2.300 peak  3251 weight  0.11000E+01 volume  0.19260E+03 ppm1     7.975 ppm2     2.971
ASSI { 3271}
   (( segid "BrD " and resid 16   and name HN  ))
   (( segid "BrD " and resid 16   and name HA  ))
      2.500     1.600     1.600 peak  3271 weight  0.11000E+01 volume  0.81267E+03 ppm1     8.792 ppm2     4.514
ASSI { 3281}
   (( segid "BrD " and resid 15   and name HN  ))
   (( segid "BrD " and resid 11   and name HA  ))
      3.600     3.200     1.900 peak  3281 weight  0.11000E+01 volume  0.88513E+02 ppm1     8.599 ppm2     4.936
ASSI { 3291}
   (( segid "BrD " and resid 15   and name HN  ))
   (( segid "BrD " and resid 15   and name HA  ))
      3.000     2.200     2.200 peak  3291 weight  0.11000E+01 volume  0.23859E+03 ppm1     8.599 ppm2     4.615
ASSI { 3301}
   (( segid "BrD " and resid 15   and name HN  ))
   (( segid "BrD " and resid 15   and name HB1 ))
      2.600     1.700     1.700 peak  3301 weight  0.11000E+01 volume  0.66455E+03 ppm1     8.598 ppm2     3.809
ASSI { 3311}
   (( segid "BrD " and resid 15   and name HN  ))
   (( segid "BrD " and resid 15   and name HB2 ))
      2.500     1.600     1.600 peak  3311 weight  0.11000E+01 volume  0.74771E+03 ppm1     8.598 ppm2     3.634
ASSI { 3331}
   (( segid "BrD " and resid 16   and name HN  ))
   (( segid "BrD " and resid 15   and name HN  ))
      2.500     1.600     1.600 peak  3331 weight  0.11000E+01 volume  0.87721E+03 ppm1     8.793 ppm2     8.628
ASSI { 3341}
   (( segid "BrD " and resid 13   and name HN  ))
   (( segid "BrD " and resid 13   and name HA  ))
      3.200     2.600     2.300 peak  3341 weight  0.11000E+01 volume  0.16876E+03 ppm1     8.801 ppm2     4.773
ASSI { 3351}
   (( segid "BrD " and resid 14   and name HN  ))
   (( segid "BrD " and resid 14   and name HA  ))
      3.200     2.700     2.200 peak  3351 weight  0.11000E+01 volume  0.15715E+03 ppm1     8.811 ppm2     4.651
ASSI { 3381}
   (( segid "BrD " and resid 13   and name HN  ))
   (( segid "BrD " and resid 13   and name HB1 ))
      2.300     1.300     1.300 peak  3381 weight  0.11000E+01 volume  0.12106E+04 ppm1     8.807 ppm2     2.758
ASSI { 3391}
   (( segid "BrD " and resid 14   and name HN  ))
   (( segid "BrD " and resid 11   and name HA  ))
      3.300     2.700     2.200 peak  3391 weight  0.11000E+01 volume  0.15172E+03 ppm1     8.809 ppm2     4.939
ASSI { 3411}
   (( segid "BrD " and resid 34   and name HN  ))
   (( segid "BrD " and resid 34   and name HA  ))
      2.800     2.000     2.000 peak  3411 weight  0.11000E+01 volume  0.39310E+03 ppm1     8.176 ppm2     5.542
ASSI { 3421}
   (( segid "BrD " and resid 34   and name HN  ))
   (( segid "BrD " and resid 34   and name HB1 ))
      3.600     3.200     1.900 peak  3421 weight  0.11000E+01 volume  0.86588E+02 ppm1     8.182 ppm2     4.098
ASSI { 3431}
   (( segid "BrD " and resid 34   and name HN  ))
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   (( segid "BrD " and resid 34   and name HB2 ))
      2.700     1.800     1.800 peak  3431 weight  0.11000E+01 volume  0.51957E+03 ppm1     8.182 ppm2     3.143
ASSI { 3441}
   (( segid "BrD " and resid 35   and name HN ))
   (( segid "BrD " and resid 34   and name HB2 ))
      3.300     2.700     2.200 peak  3441 weight  0.11000E+01 volume  0.14464E+03 ppm1     7.735 ppm2     3.139
ASSI { 3451}
   (( segid "BrD " and resid 35   and name HN ))
   (( segid "BrD " and resid 35   and name HA ))
      2.600     2.000     2.000 peak  3451 weight  0.11000E+01 volume  0.42792E+03 ppm1     7.734 ppm2     4.699
ASSI { 3461}
   (( segid "BrD " and resid 35   and name HN ))
   (( segid "BrD " and resid 35   and name HG1 ))
      2.700     1.800     1.800 peak  3461 weight  0.11000E+01 volume  0.54517E+03 ppm1     7.734 ppm2     3.436
ASSI { 3471}
   (( segid "BrD " and resid 35   and name HN ))
   (( segid "BrD " and resid 35   and name HB2 ))
      3.300     2.700     2.200 peak  3471 weight  0.11000E+01 volume  0.15293E+03 ppm1     7.733 ppm2     2.781
ASSI { 3491}
   (( segid "BrD " and resid 34   and name HN ))
   (( segid "BrD " and resid 35   and name HN ))
      2.200     1.200     1.200 peak  3491 weight  0.11000E+01 volume  0.15285E+04 ppm1     8.176 ppm2     7.714
ASSI { 3501}
   (( segid "BrD " and resid 36   and name HN ))
   (( segid "BrD " and resid 36   and name HA ))
      2.600     1.700     1.700 peak  3501 weight  0.11000E+01 volume  0.56896E+03 ppm1     8.310 ppm2     5.456
ASSI { 3511}
   (( segid "BrD " and resid 36   and name HN ))
   (( segid "BrD " and resid 36   and name HG1 ))
      3.700     3.400     1.800 peak  3511 weight  0.11000E+01 volume  0.72744E+02 ppm1     8.308 ppm2     2.771
ASSI { 3521}
   (( segid "BrD " and resid 36   and name HN ))
   (( segid "BrD " and resid 36   and name HB2 ))
      2.600     1.700     1.700 peak  3521 weight  0.11000E+01 volume  0.65455E+03 ppm1     8.311 ppm2     2.337
ASSI { 3541}
   (( segid "BrD " and resid 35   and name HN ))
   (( segid "BrD " and resid 36   and name HN ))
      2.700     1.800     1.800 peak  3541 weight  0.11000E+01 volume  0.54251E+03 ppm1     7.734 ppm2     8.316
ASSI { 3561}
   (( segid "BrD " and resid 12   and name HN ))
   (( segid "BrD " and resid 12   and name HA ))
      2.100     1.100     1.100 peak  3561 weight  0.11000E+01 volume  0.19935E+04 ppm1     9.021 ppm2     5.292
ASSI { 3571}
   (( segid "BrD " and resid 12   and name HN ))
   (( segid "BrD " and resid 12   and name HB1 ))
      2.700     1.800     1.800 peak  3571 weight  0.11000E+01 volume  0.46239E+03 ppm1     9.020 ppm2     3.428
ASSI { 3581}
   (( segid "BrD " and resid 10   and name HN ))
   (( segid "BrD " and resid 10   and name HA ))
      3.500     3.100     2.000 peak  3581 weight  0.11000E+01 volume  0.10021E+03 ppm1     8.885 ppm2     5.481
ASSI { 3591}
   (( segid "BrD " and resid 10   and name HN ))
   (( segid "BrD " and resid 10   and name HB1 ))
      3.000     2.200     2.200 peak  3591 weight  0.11000E+01 volume  0.37522E+03 ppm1     8.885 ppm2     3.361
ASSI { 3611}
   (( segid "BrD " and resid 9    and name HN ))
   (( segid "BrD " and resid 9    and name HB1 ))
      2.900     2.100     2.100 peak  3611 weight  0.11000E+01 volume  0.31864E+03 ppm1     9.054 ppm2     2.444
ASSI { 3621}
   (( segid "BrD " and resid 9    and name HN ))
   (( segid "BrD " and resid 10   and name HN ))
      3.500     3.100     2.000 peak  3621 weight  0.11000E+01 volume  0.11024E+03 ppm1     9.054 ppm2     8.880
ASSI { 3641}
   (( segid "BrD " and resid 62   and name HN ))
   (( segid "BrD " and resid 62   and name HD1 ))
      3.400     2.900     2.100 peak  3641 weight  0.11000E+01 volume  0.12186E+03 ppm1     8.998 ppm2     3.185
ASSI { 3651}
   (( segid "BrD " and resid 62   and name HN ))
   (( segid "BrD " and resid 61   and name HG2 ))
      3.000     2.200     2.200 peak  3651 weight  0.11000E+01 volume  0.24395E+03 ppm1     8.999 ppm2     2.783
ASSI { 3661}
   (( segid "BrD " and resid 62   and name HN ))
   (( segid "BrD " and resid 62   and name HG1 ))
      2.600     1.700     1.700 peak  3661 weight  0.11000E+01 volume  0.63487E+03 ppm1     8.997 ppm2     2.329
ASSI { 3681}
   (( segid "BrD " and resid 7    and name HN ))
   (( segid "BrD " and resid 7    and name HA ))
      3.100     2.400     2.400 peak  3681 weight  0.11000E+01 volume  0.21276E+03 ppm1     8.924 ppm2     5.147
ASSI { 3691}
   (( segid "BrD " and resid 7    and name HN ))
   (( segid "BrD " and resid 7    and name HG1 ))
      3.400     2.900     2.100 peak  3691 weight  0.11000E+01 volume  0.12947E+03 ppm1     8.923 ppm2     2.878
ASSI { 3701}
   (( segid "BrD " and resid 7    and name HN ))
   (( segid "BrD " and resid 7    and name HB1 ))
      3.100     2.400     2.400 peak  3701 weight  0.11000E+01 volume  0.20103E+03 ppm1     8.923 ppm2     2.631
ASSI { 3711}
   (( segid "BrD " and resid 7    and name HN ))
   (( segid "BrD " and resid 7    and name HB2 ))
      2.700     1.800     1.800 peak  3711 weight  0.11000E+01 volume  0.54229E+03 ppm1     8.924 ppm2     2.500
ASSI { 3721}
   (( segid "BrD " and resid 79   and name HN ))
   (( segid "BrD " and resid 78   and name HG ))
      2.800     2.000     2.000 peak  3721 weight  0.11000E+01 volume  0.38659E+03 ppm1     8.681 ppm2     1.314
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ASSI { 3731}
   (( segid "BrD " and resid 78   and name HN ))
   (( segid "BrD " and resid 78   and name HA ))
      2.500     1.600     1.600 peak  3731 weight  0.11000E+01 volume  0.73125E+03 ppm1     7.996 ppm2     4.004
ASSI { 3741}
   (( segid "BrD " and resid 118  and name HN ))
   (( segid "BrD " and resid 118  and name HA ))
      2.900     2.100     2.100 peak  3741 weight  0.11000E+01 volume  0.30830E+03 ppm1     8.381 ppm2     4.689
ASSI { 3761}
   (( segid "BrD " and resid 54   and name HN ))
   (( segid "BrD " and resid 54   and name HA ))
      2.900     2.100     2.100 peak  3761 weight  0.11000E+01 volume  0.30432E+03 ppm1     9.036 ppm2     5.546
ASSI { 3771}
   (( segid "BrD " and resid 54   and name HN ))
   (( segid "BrD " and resid 54   and name HB1 ))
      3.400     2.900     2.100 peak  3771 weight  0.11000E+01 volume  0.12506E+03 ppm1     9.036 ppm2     2.596
ASSI { 3781}
   (( segid "BrD " and resid 54   and name HN ))
   (( segid "BrD " and resid 54   and name HB2 ))
      3.600     3.200     1.900 peak  3781 weight  0.11000E+01 volume  0.92666E+02 ppm1     9.037 ppm2     1.960
ASSI { 3791}
   (( segid "BrD " and resid 62   and name HN ))
   (( segid "BrD " and resid 59   and name HA ))
      3.200     2.600     2.300 peak  3791 weight  0.11000E+01 volume  0.18605E+03 ppm1     8.998 ppm2     4.900
ASSI { 3801}
   (( segid "BrD " and resid 62   and name HN ))
   (( segid "BrD " and resid 62   and name HA ))
      2.800     2.000     2.000 peak  3801 weight  0.11000E+01 volume  0.36964E+03 ppm1     8.998 ppm2     4.467
ASSI { 3811}
   (( segid "BrD " and resid 72   and name HN ))
   (( segid "BrD " and resid 72   and name HA ))
      3.000     2.200     2.200 peak  3811 weight  0.11000E+01 volume  0.24473E+03 ppm1     8.858 ppm2     4.648
ASSI { 3821}
   (( segid "BrD " and resid 72   and name HN ))
   (( segid "BrD " and resid 73   and name HN ))
      3.700     3.400     1.800 peak  3821 weight  0.11000E+01 volume  0.74895E+02 ppm1     8.858 ppm2     8.033
ASSI { 3851}
   (( segid "BrD " and resid 61   and name HN ))
   (( segid "BrD " and resid 61   and name HA ))
      2.500     1.600     1.600 peak  3851 weight  0.11000E+01 volume  0.82145E+03 ppm1     8.748 ppm2     4.652
ASSI { 3861}
   (( segid "BrD " and resid 65   and name HN ))
   (( segid "BrD " and resid 62   and name HA ))
      3.100     2.400     2.400 peak  3861 weight  0.11000E+01 volume  0.22227E+03 ppm1     8.568 ppm2     4.476
ASSI { 3871}
   (( segid "BrD " and resid 60   and name HN ))
   (( segid "BrD " and resid 60   and name HA ))
      2.400     1.400     1.400 peak  3871 weight  0.11000E+01 volume  0.10791E+04 ppm1     8.569 ppm2     4.808
ASSI { 3881}
   (( segid "BrD " and resid 60   and name HN ))
   (( segid "BrD " and resid 60   and name HB2 ))
      2.400     1.400     1.400 peak  3881 weight  0.11000E+01 volume  0.10099E+04 ppm1     8.569 ppm2     4.647
ASSI { 3891}
   (( segid "BrD " and resid 60   and name HN ))
   (( segid "BrD " and resid 60   and name HB1 ))
      2.600     1.700     1.700 peak  3891 weight  0.11000E+01 volume  0.65212E+03 ppm1     8.568 ppm2     4.975
ASSI { 3901}
   (( segid "BrD " and resid 59   and name HN ))
   (( segid "BrD " and resid 59   and name HA ))
      3.200     2.600     2.300 peak  3901 weight  0.11000E+01 volume  0.18755E+03 ppm1     8.497 ppm2     4.893
ASSI { 3921}
   (( segid "BrD " and resid 7    and name HN ))
   (( segid "BrD " and resid 6    and name HA ))
      2.600     1.700     1.700 peak  3921 weight  0.11000E+01 volume  0.63166E+03 ppm1     8.924 ppm2     4.968
ASSI { 3931}
   (( segid "BrD " and resid 10   and name HN ))
   (( segid "BrD " and resid 9    and name HA ))
      2.600     1.700     1.700 peak  3931 weight  0.11000E+01 volume  0.55346E+03 ppm1     8.884 ppm2     4.938
ASSI { 3941}
   (( segid "BrD " and resid 13   and name HN ))
   (( segid "BrD " and resid 12   and name HA ))
      3.200     2.600     2.300 peak  3941 weight  0.11000E+01 volume  0.18205E+03 ppm1     8.809 ppm2     5.299
ASSI { 3951}
   (( segid "BrD " and resid 16   and name HN ))
   (( segid "BrD " and resid 15   and name HB1 ))
      3.300     2.700     2.200 peak  3951 weight  0.11000E+01 volume  0.13722E+03 ppm1     8.793 ppm2     3.818
ASSI { 3961}
   (( segid "BrD " and resid 16   and name HN ))
   (( segid "BrD " and resid 15   and name HB2 ))
      2.500     1.600     1.600 peak  3961 weight  0.11000E+01 volume  0.74092E+03 ppm1     8.793 ppm2     3.631
ASSI { 3971}
   (( segid "BrD " and resid 17   and name HN ))
   (( segid "BrD " and resid 16   and name HA ))
      2.500     1.600     1.600 peak  3971 weight  0.11000E+01 volume  0.82685E+03 ppm1     8.669 ppm2     4.516
ASSI { 3991}
   (( segid "BrD " and resid 18   and name HN ))
   (( segid "BrD " and resid 18   and name HA ))
      3.000     2.200     2.200 peak  3991 weight  0.11000E+01 volume  0.24581E+03 ppm1     9.072 ppm2     3.878
ASSI { 4001}
   (( segid "BrD " and resid 18   and name HN ))
   (( segid "BrD " and resid 17   and name HB ))
      2.800     2.000     2.000 peak  4001 weight  0.11000E+01 volume  0.36663E+03 ppm1     9.072 ppm2     4.854
ASSI { 4011}
   (( segid "BrD " and resid 18   and name HN ))
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   (( segid "BrD " and resid 17   and name HA  ))
      3.200     2.600     2.300 peak  4011 weight  0.11000E+01 volume  0.18724E+03 ppm1      9.072 ppm2      4.531
ASSI [ 4021]
   (( segid "BrD " and resid 18   and name HN  ))
   (  segid "BrD " and resid 17   and name HQ2%)
      3.100     2.400     2.400 peak  4021 weight  0.11000E+01 volume  0.33213E+03 ppm1      9.073 ppm2      1.749
ASSI [ 4041]
   (( segid "BrD " and resid 17   and name HN  ))
   (( segid "BrD " and resid 18   and name HN  ))
      2.600     1.700     1.700 peak  4041 weight  0.11000E+01 volume  0.57514E+03 ppm1      8.669 ppm2      3.062
ASSI [ 4051]
   (( segid "BrD " and resid 19   and name HN  ))
   (( segid "BrD " and resid 18   and name HA  ))
      3.500     3.100     2.000 peak  4051 weight  0.11000E+01 volume  0.95460E+02 ppm1      9.187 ppm2      3.878
ASSI [ 4061]
   (( segid "BrD " and resid 20   and name HN  ))
   (( segid "BrD " and resid 19   and name HA  ))
      3.200     2.600     2.300 peak  4061 weight  0.11000E+01 volume  0.17148E+03 ppm1      8.146 ppm2      4.288
ASSI [ 4071]
   (( segid "BrD " and resid 21   and name HN  ))
   (( segid "BrD " and resid 20   and name HA  ))
      3.400     2.900     2.100 peak  4071 weight  0.11000E+01 volume  0.11425E+03 ppm1      8.545 ppm2      4.869
ASSI [ 4081]
   (( segid "BrD " and resid 22   and name HN  ))
   (( segid "BrD " and resid 21   and name HA  ))
      3.300     2.700     2.200 peak  4081 weight  0.11000E+01 volume  0.15238E+03 ppm1      9.457 ppm2      4.361
ASSI [ 4091]
   (( segid "BrD " and resid 23   and name HN  ))
   (( segid "BrD " and resid 22   and name HA  ))
      3.600     3.200     1.900 peak  4091 weight  0.11000E+01 volume  0.91130E+02 ppm1      9.118 ppm2      4.734
ASSI [ 4101]
   (( segid "BrD " and resid 24   and name HN  ))
   (( segid "BrD " and resid 23   and name HA  ))
      3.500     3.100     2.000 peak  4101 weight  0.11000E+01 volume  0.11008E+03 ppm1      8.661 ppm2      4.640
ASSI [ 4111]
   (( segid "BrD " and resid 25   and name HN  ))
   (( segid "BrD " and resid 24   and name HA  ))
      3.300     2.700     2.200 peak  4111 weight  0.11000E+01 volume  0.14843E+03 ppm1      9.133 ppm2      4.753
ASSI [ 4121]
   (( segid "BrD " and resid 25   and name HN  ))
   (( segid "BrD " and resid 24   and name HG2 ))
      2.500     1.600     1.600 peak  4121 weight  0.11000E+01 volume  0.87462E+03 ppm1      9.131 ppm2      3.059
ASSI [ 4141]
   (( segid "BrD " and resid 27   and name HN  ))
   (( segid "BrD " and resid 26   and name HA  ))
      3.200     2.600     2.300 peak  4141 weight  0.11000E+01 volume  0.18491E+03 ppm1      8.171 ppm2      4.493
ASSI [ 4151]
   (( segid "BrD " and resid 28   and name HN  ))
   (( segid "BrD " and resid 27   and name HA  ))
      3.100     2.700     2.200 peak  4151 weight  0.11000E+01 volume  0.14739E+03 ppm1      8.166 ppm2      5.055
ASSI [ 4161]
   (( segid "BrD " and resid 29   and name HN  ))
   (( segid "BrD " and resid 28   and name HA  ))
      2.400     1.400     1.400 peak  4161 weight  0.11000E+01 volume  0.91502E+03 ppm1      9.151 ppm2      4.574
ASSI [ 4171]
   (( segid "BrD " and resid 29   and name HN  ))
   (( segid "BrD " and resid 28   and name HB1 ))
      3.400     2.900     2.100 peak  4171 weight  0.11000E+01 volume  0.11906E+03 ppm1      9.151 ppm2      3.597
ASSI [ 4181]
   (( segid "BrD " and resid 29   and name HN  ))
   (( segid "BrD " and resid 28   and name HB2 ))
      3.800     3.600     1.700 peak  4181 weight  0.11000E+01 volume  0.65813E+02 ppm1      9.152 ppm2      3.406
ASSI [ 4191]
   (( segid "BrD " and resid 30   and name HN  ))
   (( segid "BrD " and resid 29   and name HA  ))
      3.600     3.200     1.900 peak  4191 weight  0.11000E+01 volume  0.88464E+02 ppm1     12.275 ppm2      4.819
ASSI [ 4201]
   (( segid "BrD " and resid 30   and name HN  ))
   (( segid "BrD " and resid 29   and name HB1 ))
      3.400     2.900     3.100 peak  4201 weight  0.11000E+01 volume  0.11541E+03 ppm1     12.275 ppm2      2.718
ASSI [ 4211]
   (( segid "BrD " and resid 30   and name HN  ))
   (( segid "BrD " and resid 29   and name HG1 ))
      3.600     3.200     1.900 peak  4211 weight  0.11000E+01 volume  0.88536E+02 ppm1     12.275 ppm2      3.024
ASSI [ 4221]
   (( segid "BrD " and resid 31   and name HN  ))
   (( segid "BrD " and resid 30   and name HA  ))
      3.600     3.200     1.900 peak  4221 weight  0.11000E+01 volume  0.86531E+02 ppm1      8.481 ppm2      5.449
ASSI [ 4231]
   (( segid "BrD " and resid 31   and name HN  ))
   (( segid "BrD " and resid 30   and name HB1 ))
      3.000     2.200     2.200 peak  4231 weight  0.11000E+01 volume  0.23699E+03 ppm1      8.480 ppm2      4.941
ASSI [ 4241]
   (( segid "BrD " and resid 31   and name HN  ))
   (( segid "BrD " and resid 30   and name HB2 ))
      3.500     3.100     2.000 peak  4241 weight  0.11000E+01 volume  0.10932E+03 ppm1      8.480 ppm2      4.533
ASSI [ 4251]
   (( segid "BrD " and resid 66   and name HN  ))
   (( segid "BrD " and resid 67   and name HB1 ))
      2.700     1.800     1.800 peak  4251 weight  0.11000E+01 volume  0.47519E+03 ppm1      8.627 ppm2      3.555
ASSI [ 4261]
   (( segid "BrD " and resid 33   and name HN  ))
   (  segid "BrD " and resid 31   and name HB% )
      2.900     2.100     2.100 peak  4261 weight  0.11000E+01 volume  0.35188E+03 ppm1      7.739 ppm2      3.295
ASSI [ 4271]
   (( segid "BrD " and resid 32   and name HN  ))
   (( segid "BrD " and resid 31   and name HN  ))
      2.300     1.300     1.300 peak  4271 weight  0.11000E+01 volume  0.11812E+04 ppm1      7.739 ppm2      8.475
ASSI [ 4291]
   (( segid "BrD " and resid 35   and name HN  ))
   (( segid "BrD " and resid 34   and name HA  ))
      3.200     2.600     2.300 peak  4291 weight  0.11000E+01 volume  0.17960E+03 ppm1      7.734 ppm2      5.537
ASSI [ 4301]
   (( segid "BrD " and resid 36   and name HN  ))
   (( segid "BrD " and resid 37   and name HD1 ))
      3.500     3.100     2.000 peak  4301 weight  0.11000E+01 volume  0.97101E+02 ppm1      8.309 ppm2      4.277
ASSI [ 4311]
   (( segid "BrD " and resid 36   and name HN  ))
   (( segid "BrD " and resid 35   and name HA  ))
      3.300     2.700     2.300 peak  4311 weight  0.11000E+01 volume  0.16106E+03 ppm1      8.308 ppm2      4.893
ASSI [ 4321]
   (( segid "BrD " and resid 36   and name HN  ))
   (( segid "BrD " and resid 35   and name HG1 ))
      3.700     3.400     1.800 peak  4321 weight  0.11000E+01 volume  0.78555E+02 ppm1      8.307 ppm2      3.458
ASSI [ 4331]
   (( segid "BrD " and resid 39   and name HN  ))
   (( segid "BrD " and resid 38   and name HA  ))
      3.200     1.200     1.200 peak  4331 weight  0.11000E+01 volume  0.15683E+04 ppm1      9.652 ppm2      4.160
ASSI [ 4341]
   (( segid "BrD " and resid 39   and name HN  ))
   (( segid "BrD " and resid 38   and name HB  ))
      3.400     2.900     2.100 peak  4341 weight  0.11000E+01 volume  0.11939E+03 ppm1      9.652 ppm2      1.752
ASSI [ 4351]
   (( segid "BrD " and resid 39   and name HN  ))
   (  segid "BrD " and resid 38   and name HG1%)
      3.400     3.200     1.900 peak  4351 weight  0.11000E+01 volume  0.93234E+02 ppm1      9.652 ppm2      1.071
ASSI [ 4361]
   (( segid "BrD " and resid 39   and name HN  ))
   (  segid "BrD " and resid 38   and name HG2%)
      3.100     2.400     2.400 peak  4361 weight  0.11000E+01 volume  0.20061E+03 ppm1      9.652 ppm2      0.776
ASSI [ 4381]
   (( segid "BrD " and resid 43   and name HN  ))
   (( segid "BrD " and resid 42   and name HA  ))
      2.900     2.100     2.100 peak  4381 weight  0.11000E+01 volume  0.31681E+03 ppm1      8.001 ppm2      5.055
ASSI [ 4391]
   (( segid "BrD " and resid 43   and name HN  ))
   (( segid "BrD " and resid 42   and name HB2 ))
      2.800     2.000     2.000 peak  4391 weight  0.11000E+01 volume  0.36989E+03 ppm1      8.001 ppm2      2.607
ASSI [ 4401]
   (( segid "BrD " and resid 43   and name HN  ))
   (( segid "BrD " and resid 42   and name HB1 ))
      2.900     2.100     2.100 peak  4401 weight  0.11000E+01 volume  0.32280E+03 ppm1      8.001 ppm2      2.781
ASSI [ 4411]
   (( segid "BrD " and resid 36   and name HN  ))
   (( segid "BrD " and resid 36   and name HB1 ))
      2.800     2.000     2.000 peak  4411 weight  0.11000E+01 volume  0.42122E+03 ppm1      8.308 ppm2      2.698
ASSI [ 4421]
   (( segid "BrD " and resid 47   and name HN  ))
   (( segid "BrD " and resid 46   and name HA  ))
      3.300     2.700     2.200 peak  4421 weight  0.11000E+01 volume  0.14320E+03 ppm1      8.832 ppm2      4.139
ASSI [ 4431]
   (( segid "BrD " and resid 47   and name HN  ))
   (( segid "BrD " and resid 46   and name HB1 ))
      3.500     3.100     2.000 peak  4431 weight  0.11000E+01 volume  0.11013E+03 ppm1      8.832 ppm2      3.296
ASSI [ 4441]
   (( segid "BrD " and resid 47   and name HN  ))
   (( segid "BrD " and resid 46   and name HB2 ))
      3.100     2.400     2.400 peak  4441 weight  0.11000E+01 volume  0.20297E+03 ppm1      8.833 ppm2      3.094
ASSI [ 4451]
   (( segid "BrD " and resid 48   and name HN  ))
   (( segid "BrD " and resid 47   and name HA  ))
      3.200     2.600     2.300 peak  4451 weight  0.11000E+01 volume  0.16849E+03 ppm1      8.307 ppm2      4.708
ASSI [ 4461]
   (( segid "BrD " and resid 49   and name HN  ))
   (( segid "BrD " and resid 48   and name HA  ))
      3.000     2.200     2.200 peak  4461 weight  0.11000E+01 volume  0.24376E+03 ppm1      7.762 ppm2      4.816
ASSI [ 4471]
   (( segid "BrD " and resid 49   and name HN  ))
   (( segid "BrD " and resid 48   and name HG2 ))
      4.000     4.000     1.500 peak  4471 weight  0.11000E+01 volume  0.45461E+02 ppm1      7.762 ppm2      2.872
ASSI [ 4481]
   (( segid "BrD " and resid 49   and name HN  ))
   (( segid "BrD " and resid 48   and name HB1 ))
      3.200     2.600     2.300 peak  4481 weight  0.11000E+01 volume  0.17937E+03 ppm1      7.762 ppm2      2.693
ASSI [ 4491]
   (( segid "BrD " and resid 50   and name HN  ))
   (( segid "BrD " and resid 49   and name HA  ))
      2.600     1.700     1.700 peak  4491 weight  0.11000E+01 volume  0.60014E+03 ppm1      8.564 ppm2      4.693
ASSI [ 4501]
   (( segid "BrD " and resid 50   and name HN  ))
   (( segid "BrD " and resid 49   and name HB  ))
      2.900     2.100     2.100 peak  4501 weight  0.11000E+01 volume  0.31627E+03 ppm1      8.564 ppm2      2.622
ASSI [ 4511]
   (( segid "BrD " and resid 50   and name HN  ))
   (  segid "BrD " and resid 49   and name HG2%)
      3.700     3.400     1.800 peak  4511 weight  0.11000E+01 volume  0.77577E+02 ppm1      8.564 ppm2      1.598
ASSI [ 4521]
   (( segid "BrD " and resid 58   and name HN  ))
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   (( segid "BrD " and resid 54   and name HA  ))
      2.300     1.300     1.300 peak  4521 weight  0.11000E+01 volume  0.11556E+04 ppm1      7.974 ppm2      5.542
ASSI [ 4531]
   (( segid "BrD " and resid 55   and name HN  ))
   (( segid "BrD " and resid 54   and name HB1 ))
      3.700     1.400     1.800 peak  4531 weight  0.11000E+01 volume  0.71474E+02 ppm1      7.975 ppm2      2.572
ASSI [ 4541]
   (( segid "BrD " and resid 55   and name HN  ))
   (( segid "BrD " and resid 54   and name HB2 ))
      3.100     2.400     2.400 peak  4541 weight  0.11000E+01 volume  0.20373E+03 ppm1      7.975 ppm2      1.956
ASSI [ 4551]
   (( segid "BrD " and resid 56   and name HN  ))
   (( segid "BrD " and resid 55   and name HA  ))
      2.800     2.000     2.000 peak  4551 weight  0.11000E+01 volume  0.38353E+03 ppm1      9.676 ppm2      5.352
ASSI [ 4561]
   (( segid "BrD " and resid 56   and name HN  ))
   (( segid "BrD " and resid 55   and name HB1 ))
      2.400     1.400     1.400 peak  4561 weight  0.11000E+01 volume  0.92127E+03 ppm1      9.679 ppm2      2.978
ASSI [ 4571]
   (( segid "BrD " and resid 57   and name HN  ))
   (( segid "BrD " and resid 56   and name HA  ))
      3.200     2.600     2.300 peak  4571 weight  0.11000E+01 volume  0.16116E+03 ppm1      9.359 ppm2      4.648
ASSI [ 4581]
   (( segid "BrD " and resid 58   and name HN  ))
   (( segid "BrD " and resid 57   and name HA  ))
      3.400     2.900     2.100 peak  4581 weight  0.11000E+01 volume  0.12185E+03 ppm1     10.050 ppm2      4.805
ASSI [ 4591]
   (( segid "BrD " and resid 59   and name HN  ))
   (( segid "BrD " and resid 58   and name HA  ))
      3.400     2.900     2.100 peak  4591 weight  0.11000E+01 volume  0.13191E+03 ppm1      8.498 ppm2      4.449
ASSI [ 4601]
   (( segid "BrD " and resid 59   and name HN  ))
   (( segid "BrD " and resid 58   and name HB  ))
      3.200     2.600     2.300 peak  4601 weight  0.11000E+01 volume  0.18613E+03 ppm1      8.498 ppm2      4.697
ASSI [ 4611]
   (( segid "BrD " and resid 59   and name HN  ))
   (  segid "BrD " and resid 58   and name HG2% )
      3.100     2.400     2.400 peak  4611 weight  0.11000E+01 volume  0.21128E+03 ppm1      8.496 ppm2      1.665
ASSI [ 4621]
   (( segid "BrD " and resid 58   and name HN  ))
   (( segid "BrD " and resid 59   and name HN  ))
      3.200     2.600     2.300 peak  4621 weight  0.11000E+01 volume  0.17034E+03 ppm1     10.051 ppm2      8.489
ASSI [ 4641]
   (( segid "BrD " and resid 61   and name HN  ))
   (( segid "BrD " and resid 61   and name HG1 ))
      2.400     1.400     1.400 peak  4641 weight  0.11000E+01 volume  0.89496E+03 ppm1      8.743 ppm2      2.974
ASSI [ 4651]
   (( segid "BrD " and resid 61   and name HN  ))
   (( segid "BrD " and resid 61   and name HB2 ))
      2.500     1.400     1.600 peak  4651 weight  0.11000E+01 volume  0.72876E+03 ppm1      8.743 ppm2      2.670
ASSI [ 4661]
   (( segid "BrD " and resid 61   and name HN  ))
   (( segid "BrD " and resid 60   and name HA  ))
      3.300     2.700     2.200 peak  4661 weight  0.11000E+01 volume  0.14220E+03 ppm1      8.749 ppm2      4.816
ASSI [ 4691]
   (( segid "BrD " and resid 60   and name HN  ))
   (( segid "BrD " and resid 61   and name HN  ))
      2.400     1.400     1.400 peak  4691 weight  0.11000E+01 volume  0.96369E+03 ppm1      8.566 ppm2      8.734
ASSI [ 4701]
   (( segid "BrD " and resid 62   and name HN  ))
   (( segid "BrD " and resid 61   and name HA  ))
      3.200     2.600     2.300 peak  4701 weight  0.11000E+01 volume  0.17192E+03 ppm1      8.997 ppm2      4.656
ASSI [ 4711]
   (( segid "BrD " and resid 63   and name HN  ))
   (( segid "BrD " and resid 62   and name HN  ))
      2.800     2.000     2.000 peak  4711 weight  0.11000E+01 volume  0.35764E+03 ppm1      9.477 ppm2      8.998
ASSI [ 4731]
   (( segid "BrD " and resid 63   and name HN  ))
   (( segid "BrD " and resid 62   and name HA  ))
      3.600     3.200     1.900 peak  4731 weight  0.11000E+01 volume  0.90728E+02 ppm1      9.472 ppm2      4.481
ASSI [ 4741]
   (( segid "BrD " and resid 65   and name HD21))
   (( segid "BrD " and resid 65   and name HB1 ))
      3.500     3.100     2.000 peak  4741 weight  0.11000E+01 volume  0.10454E+03 ppm1      8.206 ppm2      3.637
ASSI [ 4751]
   (( segid "BrD " and resid 65   and name HD22))
   (( segid "BrD " and resid 65   and name HB1 ))
      3.500     3.100     2.000 peak  4751 weight  0.11000E+01 volume  0.97769E+02 ppm1      7.576 ppm2      3.637
ASSI [ 4761]
   (( segid "BrD " and resid 65   and name HD21))
   (( segid "BrD " and resid 65   and name HB2 ))
      3.200     2.600     2.300 peak  4761 weight  0.11000E+01 volume  0.17538E+03 ppm1      8.205 ppm2      3.393
ASSI [ 4771]
   (( segid "BrD " and resid 65   and name HD22))
   (( segid "BrD " and resid 65   and name HB2 ))
      3.400     2.900     2.100 peak  4771 weight  0.11000E+01 volume  0.13182E+03 ppm1      7.576 ppm2      3.393
ASSI [ 4781]
   (( segid "BrD " and resid 24   and name HE21))
   (( segid "BrD " and resid 24   and name HG1 ))
      3.400     2.900     2.100 peak  4781 weight  0.11000E+01 volume  0.11561E+03 ppm1      7.634 ppm2      3.459
ASSI [ 4791]
   (( segid "BrD " and resid 24   and name HE22))
   (( segid "BrD " and resid 24   and name HG1 ))
      3.600     3.200     1.900 peak  4791 weight  0.11000E+01 volume  0.90206E+02 ppm1      7.533 ppm2      3.474
ASSI [ 4801]
   (( segid "BrD " and resid 66   and name HN  ))
   (( segid "BrD " and resid 65   and name HA  ))
      2.700     1.800     1.800 peak  4801 weight  0.11000E+01 volume  0.48146E+03 ppm1      8.763 ppm2      5.378
ASSI [ 4811]
   (( segid "BrD " and resid 66   and name HN  ))
   (( segid "BrD " and resid 65   and name HB1 ))
      3.400     2.900     2.100 peak  4811 weight  0.11000E+01 volume  0.11537E+03 ppm1      8.759 ppm2      3.608
ASSI [ 4821]
   (( segid "BrD " and resid 66   and name HN  ))
   (( segid "BrD " and resid 65   and name HB2 ))
      3.300     2.700     2.200 peak  4821 weight  0.11000E+01 volume  0.13853E+03 ppm1      8.763 ppm2      3.381
ASSI [ 4831]
   (( segid "BrD " and resid 67   and name HN  ))
   (( segid "BrD " and resid 66   and name HA  ))
      2.800     3.000     2.000 peak  4831 weight  0.11000E+01 volume  0.41855E+03 ppm1      8.832 ppm2      5.009
ASSI [ 4841]
   (( segid "BrD " and resid 68   and name HN  ))
   (( segid "BrD " and resid 67   and name HA  ))
      3.400     2.900     2.100 peak  4841 weight  0.11000E+01 volume  0.12732E+03 ppm1      8.627 ppm2      4.671
ASSI [ 4851]
   (( segid "BrD " and resid 68   and name HN  ))
   (( segid "BrD " and resid 67   and name HB2 ))
      3.300     2.700     2.200 peak  4851 weight  0.11000E+01 volume  0.15213E+03 ppm1      8.626 ppm2      2.662
ASSI [ 4861]
   (( segid "BrD " and resid 69   and name HN  ))
   (( segid "BrD " and resid 68   and name HA  ))
      2.400     1.400     1.400 peak  4861 weight  0.11000E+01 volume  0.95815E+03 ppm1      8.305 ppm2      5.161
ASSI [ 4871]
   (( segid "BrD " and resid 69   and name HN  ))
   (( segid "BrD " and resid 68   and name HB1 ))
      4.500     4.900     1.000 peak  4871 weight  0.11000E+01 volume  0.22391E+02 ppm1      8.306 ppm2      3.669
ASSI [ 4881]
   (( segid "BrD " and resid 69   and name HN  ))
   (( segid "BrD " and resid 68   and name HB2 ))
      3.300     2.700     2.200 peak  4881 weight  0.11000E+01 volume  0.15981E+03 ppm1      8.306 ppm2      3.514
ASSI [ 4891]
   (( segid "BrD " and resid 70   and name HN  ))
   (( segid "BrD " and resid 69   and name HA  ))
      3.000     2.200     2.200 peak  4891 weight  0.11000E+01 volume  0.24443E+03 ppm1      8.039 ppm2      4.690
ASSI [ 4901]
   (( segid "BrD " and resid 70   and name HN  ))
   (( segid "BrD " and resid 69   and name HB  ))
      3.400     2.900     2.100 peak  4901 weight  0.11000E+01 volume  0.12954E+03 ppm1      8.040 ppm2      2.928
ASSI [ 4911]
   (( segid "BrD " and resid 70   and name HN  ))
   (  segid "BrD " and resid 69   and name HG1% )
      3.800     3.600     1.700 peak  4911 weight  0.11000E+01 volume  0.61869E+02 ppm1      8.041 ppm2      1.551
ASSI [ 4921]
   (( segid "BrD " and resid 70   and name HN  ))
   (  segid "BrD " and resid 69   and name HG2% )
      2.700     1.800     1.800 peak  4921 weight  0.11000E+01 volume  0.48346E+03 ppm1      8.040 ppm2      1.430
ASSI [ 4931]
   (( segid "BrD " and resid 73   and name HN  ))
   (( segid "BrD " and resid 72   and name HA  ))
      2.900     2.100     2.100 peak  4931 weight  0.11000E+01 volume  0.30696E+03 ppm1      8.045 ppm2      4.654
ASSI [ 4941]
   (( segid "BrD " and resid 74   and name HN  ))
   (( segid "BrD " and resid 73   and name HA  ))
      3.500     3.100     2.000 peak  4941 weight  0.11000E+01 volume  0.10430E+03 ppm1      7.536 ppm2      4.812
ASSI [ 4951]
   (( segid "BrD " and resid 75   and name HN  ))
   (( segid "BrD " and resid 74   and name HA  ))
      3.500     3.100     2.000 peak  4951 weight  0.11000E+01 volume  0.10099E+03 ppm1      9.106 ppm2      4.361
ASSI [ 4961]
   (( segid "BrD " and resid 76   and name HN  ))
   (( segid "BrD " and resid 75   and name HA  ))
      3.400     2.900     2.100 peak  4961 weight  0.11000E+01 volume  0.11734E+03 ppm1      8.611 ppm2      4.525
ASSI [ 4971]
   (( segid "BrD " and resid 76   and name HN  ))
   (( segid "BrD " and resid 75   and name HG1 ))
      3.000     2.200     2.200 peak  4971 weight  0.11000E+01 volume  0.28328E+03 ppm1      8.611 ppm2      3.549
ASSI [ 4981]
   (( segid "BrD " and resid 76   and name HN  ))
   (( segid "BrD " and resid 75   and name HG2 ))
      3.200     2.600     2.300 peak  4981 weight  0.11000E+01 volume  0.18815E+03 ppm1      8.610 ppm2      3.218
ASSI [ 4991]
   (( segid "BrD " and resid 76   and name HN  ))
   (( segid "BrD " and resid 75   and name HB2 ))
      2.600     1.700     1.700 peak  4991 weight  0.11000E+01 volume  0.61964E+03 ppm1      8.611 ppm2      2.815
ASSI [ 5001]
   (( segid "BrD " and resid 76   and name HN  ))
   (( segid "BrD " and resid 75   and name HB1 ))
      2.600     1.700     1.700 peak  5001 weight  0.11000E+01 volume  0.59739E+03 ppm1      8.611 ppm2      2.925
ASSI [ 5011]
   (( segid "BrD " and resid 77   and name HN  ))
   (( segid "BrD " and resid 76   and name HA  ))
      3.000     2.200     2.200 peak  5011 weight  0.11000E+01 volume  0.25554E+03 ppm1      7.996 ppm2      4.695
ASSI [ 5021]
   (( segid "BrD " and resid 77   and name HN  ))
   (  segid "BrD " and resid 76   and name HB% )
      2.500     1.600     1.600 peak  5021 weight  0.11000E+01 volume  0.86259E+03 ppm1      7.996 ppm2      2.092
ASSI [ 5031]
   (( segid "BrD " and resid 79   and name HN  ))
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   (( segid "BrD " and resid 78   and name HA  ))
      3.300     2.700     2.200 peak  5031 weight  0.11000E+01 volume  0.14659E+03 ppm1    8.681 ppm2    3.995
ASSI { 5041}
   (( segid "BrD " and resid 78   and name HN  ))
   (( segid "BrD " and resid 79   and name HN  ))
      2.400     1.400     1.400 peak  5041 weight  0.11000E+01 volume  0.10403E+04 ppm1    7.996 ppm2    8.687
ASSI { 5061}
   (( segid "BrD " and resid 80   and name HN  ))
   (( segid "BrD " and resid 80   and name HD1 ))
      5.300     5.300     0.200 peak  5061 weight  0.11000E+01 volume  0.85899E+01 ppm1    8.006 ppm2    3.997
ASSI { 5071}
   (( segid "BrD " and resid 80   and name HN  ))
   (( segid "BrD " and resid 79   and name HA  ))
      3.300     2.700     2.200 peak  5071 weight  0.11000E+01 volume  0.15955E+03 ppm1    8.006 ppm2    4.404
ASSI { 5091}
   (( segid "BrD " and resid 80   and name HN  ))
   (( segid "BrD " and resid 79   and name HB2 ))
      3.200     2.600     2.300 peak  5091 weight  0.11000E+01 volume  0.16421E+03 ppm1    8.006 ppm2    2.704
ASSI { 5101}
   (( segid "BrD " and resid 81   and name HN  ))
   (( segid "BrD " and resid 80   and name HA  ))
      3.700     3.400     1.800 peak  5101 weight  0.11000E+01 volume  0.77456E+02 ppm1    7.639 ppm2    4.685
ASSI { 5111}
   (( segid "BrD " and resid 82   and name HN  ))
   (( segid "BrD " and resid 81   and name HB  ))
      2.500     1.600     1.600 peak  5111 weight  0.11000E+01 volume  0.81882E+03 ppm1    6.981 ppm2    2.042
ASSI { 5121}
   (( segid "BrD " and resid 82   and name HN  ))
   (  segid "BrD " and resid 81   and name HG1%)
      3.200     2.600     2.300 peak  5121 weight  0.11000E+01 volume  0.17066E+03 ppm1    6.981 ppm2    1.086
ASSI { 5131}
   (( segid "BrD " and resid 82   and name HN  ))
   (  segid "BrD " and resid 81   and name HG2%)
      3.400     2.900     2.100 peak  5131 weight  0.11000E+01 volume  0.12101E+03 ppm1    6.981 ppm2    0.749
ASSI { 5141}
   (( segid "BrD " and resid 83   and name HN  ))
   (( segid "BrD " and resid 82   and name HA  ))
      3.400     2.900     2.100 peak  5141 weight  0.11000E+01 volume  0.11364E+03 ppm1    9.658 ppm2    4.743
ASSI { 5151}
   (( segid "BrD " and resid 83   and name HN  ))
   (( segid "BrD " and resid 82   and name HB1 ))
      3.500     3.100     2.000 peak  5151 weight  0.11000E+01 volume  0.10752E+03 ppm1    9.660 ppm2    3.697
ASSI { 5161}
   (( segid "BrD " and resid 83   and name HN  ))
   (( segid "BrD " and resid 82   and name HB2 ))
      2.800     2.000     2.000 peak  5161 weight  0.11000E+01 volume  0.41394E+03 ppm1    9.658 ppm2    3.551
ASSI { 5171}
   (( segid "BrD " and resid 84   and name HN  ))
   (( segid "BrD " and resid 83   and name HB  ))
      3.200     2.600     2.300 peak  5171 weight  0.11000E+01 volume  0.19086E+03 ppm1    9.466 ppm2    4.817
ASSI { 5181}
   (( segid "BrD " and resid 84   and name HN  ))
   (( segid "BrD " and resid 83   and name HA  ))
      3.600     3.200     1.900 peak  5181 weight  0.11000E+01 volume  0.83498E+02 ppm1    9.463 ppm2    4.449
ASSI { 5191}
   (( segid "BrD " and resid 84   and name HN  ))
   (  segid "BrD " and resid 83   and name HG2%)
      3.500     3.100     2.000 peak  5191 weight  0.11000E+01 volume  0.11050E+03 ppm1    9.463 ppm2    1.903
ASSI { 5201}
   (( segid "BrD " and resid 85   and name HN  ))
   (( segid "BrD " and resid 84   and name HA  ))
      3.700     3.400     1.800 peak  5201 weight  0.11000E+01 volume  0.79848E+02 ppm1    7.515 ppm2    4.921
ASSI { 5211}
   (( segid "BrD " and resid 85   and name HN  ))
   (( segid "BrD " and resid 84   and name HB2 ))
      3.400     2.900     2.100 peak  5211 weight  0.11000E+01 volume  0.12439E+03 ppm1    7.516 ppm2    3.268
ASSI { 5221}
   (( segid "BrD " and resid 86   and name HN  ))
   (( segid "BrD " and resid 85   and name HA  ))
      3.900     3.800     1.600 peak  5221 weight  0.11000E+01 volume  0.50221E+02 ppm1    8.423 ppm2    5.012
ASSI { 5231}
   (( segid "BrD " and resid 86   and name HN  ))
   (( segid "BrD " and resid 85   and name HB2 ))
      3.300     2.700     2.200 peak  5231 weight  0.11000E+01 volume  0.14503E+03 ppm1    8.423 ppm2    3.639
ASSI { 5241}
   (( segid "BrD " and resid 87   and name HN  ))
   (( segid "BrD " and resid 86   and name HA  ))
      3.600     3.200     1.900 peak  5241 weight  0.11000E+01 volume  0.84494E+02 ppm1    8.572 ppm2    4.815
ASSI { 5251}
   (( segid "BrD " and resid 88   and name HN  ))
   (( segid "BrD " and resid 87   and name HA  ))
      3.600     3.200     1.900 peak  5251 weight  0.11000E+01 volume  0.87457E+02 ppm1    8.357 ppm2    4.657
ASSI { 5261}
   (( segid "BrD " and resid 88   and name HN  ))
   (( segid "BrD " and resid 87   and name HB1 ))
      3.100     2.400     2.400 peak  5261 weight  0.11000E+01 volume  0.23456E+03 ppm1    8.354 ppm2    2.782
ASSI { 5271}
   (( segid "BrD " and resid 88   and name HN  ))
   (( segid "BrD " and resid 87   and name HB2 ))
      3.200     2.600     2.300 peak  5271 weight  0.11000E+01 volume  0.19424E+03 ppm1    8.354 ppm2    2.614
ASSI { 5281}
   (( segid "BrD " and resid 88   and name HN  ))
   (( segid "BrD " and resid 87   and name HN  ))
      2.400     1.700     1.700 peak  5281 weight  0.11000E+01 volume  0.67695E+03 ppm1    8.355 ppm2    8.552
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ASSI { 5301}
   (( segid "BrD " and resid 89   and name HN  ))
   (( segid "BrD " and resid 88   and name HA  ))
      3.400     2.900     2.100 peak  5301 weight  0.11000E+01 volume  0.12542E+03 ppm1    8.858 ppm2    4.976
ASSI { 5311}
   (( segid "BrD " and resid 89   and name HD21))
   (( segid "BrD " and resid 89   and name HB2 ))
      3.900     3.800     1.600 peak  5311 weight  0.11000E+01 volume  0.54504E+02 ppm1    8.923 ppm2    3.516
ASSI { 5321}
   (( segid "BrD " and resid 89   and name HD22))
   (( segid "BrQ " and resid 89   and name HB2 ))
      3.300     2.700     2.200 peak  5321 weight  0.11000E+01 volume  0.13631E+03 ppm1    8.416 ppm2    3.514
ASSI { 5331}
   (( segid "BrD " and resid 89   and name HD21))
   (( segid "BrD " and resid 89   and name HB1 ))
      5.100     5.100     0.400 peak  5331 weight  0.11000E+01 volume  0.10399E+02 ppm1    8.923 ppm2    3.679
ASSI { 5341}
   (( segid "BrD " and resid 89   and name HD22))
   (( segid "BrD " and resid 89   and name HB1 ))
      3.900     3.800     1.600 peak  5341 weight  0.11000E+01 volume  0.50137E+02 ppm1    8.416 ppm2    3.676
ASSI { 5351}
   (( segid "BrD " and resid 92   and name HN  ))
   (( segid "BrD " and resid 93   and name HG1 ))
      2.700     1.800     1.800 peak  5351 weight  0.11000E+01 volume  0.53011E+03 ppm1    8.876 ppm2    2.818
ASSI { 5361}
   (( segid "BrD " and resid 92   and name HN  ))
   (( segid "BrD " and resid 92   and name HB1 ))
      3.600     3.200     1.900 peak  5361 weight  0.11000E+01 volume  0.93226E+02 ppm1    8.875 ppm2    2.697
ASSI { 5371}
   (( segid "BrD " and resid 92   and name HN  ))
   (( segid "BrD " and resid 92   and name HB2 ))
      2.500     1.600     1.600 peak  5371 weight  0.11000E+01 volume  0.87608E+03 ppm1    8.875 ppm2    2.576
ASSI { 5381}
   (( segid "BrD " and resid 93   and name HN  ))
   (( segid "BrD " and resid 92   and name HG1 ))
      3.500     3.100     2.000 peak  5381 weight  0.11000E+01 volume  0.10524E+03 ppm1    8.714 ppm2    2.807
ASSI { 5391}
   (( segid "BrD " and resid 93   and name HN  ))
   (( segid "BrD " and resid 92   and name HB1 ))
      3.200     2.600     2.300 peak  5391 weight  0.11000E+01 volume  0.16925E+03 ppm1    8.714 ppm2    2.702
ASSI { 5401}
   (( segid "BrD " and resid 93   and name HN  ))
   (( segid "BrD " and resid 92   and name HB2 ))
      3.300     2.700     2.200 peak  5401 weight  0.11000E+01 volume  0.13613E+03 ppm1    8.714 ppm2    3.560
ASSI { 5411}
   (( segid "BrD " and resid 94   and name HN  ))
   (( segid "BrD " and resid 94   and name HB1 ))
      2.700     1.800     1.800 peak  5411 weight  0.11000E+01 volume  0.51785E+03 ppm1    9.677 ppm2    2.777
ASSI { 5421}
   (( segid "BrD " and resid 94   and name HN  ))
   (( segid "BrD " and resid 94   and name HG1 ))
      3.600     3.200     1.900 peak  5421 weight  0.11000E+01 volume  0.85031E+02 ppm1    9.679 ppm2    3.144
ASSI { 5431}
   (( segid "BrD " and resid 94   and name HN  ))
   (( segid "BrD " and resid 93   and name HA  ))
      3.300     2.700     2.200 peak  5431 weight  0.11000E+01 volume  0.15969E+03 ppm1    9.678 ppm2    3.042
ASSI { 5441}
   (( segid "BrD " and resid 94   and name HN  ))
   (( segid "BrD " and resid 93   and name HB2 ))
      3.000     2.200     2.200 peak  5441 weight  0.11000E+01 volume  0.25357E+03 ppm1    9.680 ppm2    4.764
ASSI { 5451}
   (( segid "BrD " and resid 95   and name HN  ))
   (( segid "BrD " and resid 94   and name HA  ))
      3.600     3.200     1.900 peak  5451 weight  0.11000E+01 volume  0.81131E+02 ppm1    8.669 ppm2    4.839
ASSI { 5461}
   (( segid "BrD " and resid 95   and name HN  ))
   (( segid "BrD " and resid 94   and name HG1 ))
      3.400     2.900     2.100 peak  5461 weight  0.11000E+01 volume  0.12127E+03 ppm1    8.669 ppm2    3.135
ASSI { 5471}
   (( segid "BrD " and resid 95   and name HN  ))
   (( segid "BrD " and resid 94   and name HB1 ))
      2.800     2.000     2.000 peak  5471 weight  0.11000E+01 volume  0.41579E+03 ppm1    8.670 ppm2    3.776
ASSI { 5481}
   (( segid "BrD " and resid 96   and name HN  ))
   (( segid "BrD " and resid 95   and name HN  ))
      2.400     1.400     1.400 peak  5481 weight  0.11000E+01 volume  0.91814E+03 ppm1    7.979 ppm2    8.679
ASSI { 5501}
   (( segid "BrD " and resid 97   and name HN  ))
   (( segid "BrD " and resid 96   and name HA  ))
      3.300     2.700     2.200 peak  5501 weight  0.11000E+01 volume  0.15786E+03 ppm1    8.677 ppm2    4.426
ASSI { 5511}
   (( segid "BrD " and resid 97   and name HN  ))
   (( segid "BrD " and resid 96   and name HB1 ))
      3.200     2.600     2.300 peak  5511 weight  0.11000E+01 volume  0.17339E+03 ppm1    8.674 ppm2    3.997
ASSI { 5521}
   (( segid "BrD " and resid 97   and name HN  ))
   (( segid "BrD " and resid 96   and name HB2 ))
      3.000     2.200     2.200 peak  5521 weight  0.11000E+01 volume  0.24046E+03 ppm1    8.674 ppm2    3.107
ASSI { 5531}
   (( segid "BrD " and resid 99   and name HN  ))
   (( segid "BrD " and resid 98   and name HA  ))
      3.200     2.600     2.300 peak  5531 weight  0.11000E+01 volume  0.16965E+03 ppm1    8.936 ppm2    4.813
ASSI { 5541}
   (( segid "BrD " and resid 99   and name HN  ))
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   (( segid "BrD " and resid 98   and name HB1 ))
      3.200      2.600      2.300 peak   5541 weight  0.11000E+01 volume  0.16699E+03 ppm1      8.936 ppm2      4.003
 ASSI [ 5551]
   (( segid "BrD " and resid 99   and name HN  ))
   (( segid "BrD " and resid 98   and name HB2 ))
      2.900      2.100      2.100 peak   5551 weight  0.11000E+01 volume  0.29941E+03 ppm1      8.936 ppm2      3.663
 ASSI [ 5561]
   (( segid "BrD " and resid 100  and name HN  ))
   (( segid "BrD " and resid 99   and name HA  ))
      3.300      2.700      2.200 peak   5561 weight  0.11000E+01 volume  0.14856E+03 ppm1      8.669 ppm2      4.438
 ASSI [ 5571]
   (( segid "BrD " and resid 100  and name HN  ))
   (  segid "BrD " and resid 99   and name HB% )
      2.600      1.700      1.700 peak   5571 weight  0.11000E+01 volume  0.56660E+03 ppm1      8.669 ppm2      2.204
 ASSI [ 5581]
   (( segid "BrD " and resid 101  and name HN  ))
   (( segid "BrD " and resid 100  and name HA  ))
      3.500      3.100      2.000 peak   5581 weight  0.11000E+01 volume  0.99135E+02 ppm1      8.513 ppm2      4.940
 ASSI [ 5591]
   (( segid "BrD " and resid 101  and name HN  ))
   (( segid "BrD " and resid 100  and name HB1 ))
      3.200      2.600      2.300 peak   5591 weight  0.11000E+01 volume  0.18321E+03 ppm1      8.513 ppm2      3.484
 ASSI [ 5601]
   (( segid "BrD " and resid 102  and name HN  ))
   (( segid "BrD " and resid 101  and name HA  ))
      3.500      3.100      2.000 peak   5601 weight  0.11000E+01 volume  0.10380E+03 ppm1      9.156 ppm2      4.256
 ASSI [ 5611]
   (( segid "BrD " and resid 103  and name HN  ))
   (( segid "BrD " and resid 102  and name HA  ))
      3.500      3.100      2.000 peak   5611 weight  0.11000E+01 volume  0.10037E+03 ppm1      8.696 ppm2      4.277
 ASSI [ 5621]
   (( segid "BrD " and resid 104  and name HN  ))
   (( segid "BrD " and resid 103  and name HA  ))
      3.200      2.600      2.300 peak   5621 weight  0.11000E+01 volume  0.16539E+03 ppm1      7.763 ppm2      3.792
 ASSI [ 5631]
   (( segid "BrD " and resid 104  and name HN  ))
   (( segid "BrD " and resid 103  and name HB1 ))
      2.800      2.000      2.000 peak   5631 weight  0.11000E+01 volume  0.39404E+03 ppm1      7.762 ppm2      2.327
 ASSI [ 5641]
   (( segid "BrD " and resid 104  and name HN  ))
   (( segid "BrD " and resid 103  and name HB2 ))
      3.200      2.600      2.300 peak   5641 weight  0.11000E+01 volume  0.16250E+03 ppm1      7.763 ppm2      1.917
 ASSI [ 5651]
   (( segid "BrD " and resid 105  and name HN  ))
   (( segid "BrD " and resid 104  and name HA  ))
      3.200      2.600      2.300 peak   5651 weight  0.11000E+01 volume  0.16160E+03 ppm1      8.488 ppm2      4.668
 ASSI [ 5661]
   (( segid "BrD " and resid 106  and name HN  ))
   (( segid "BrD " and resid 105  and name HA  ))
      3.600      3.200      1.900 peak   5661 weight  0.11000E+01 volume  0.94653E+02 ppm1      9.740 ppm2      4.934
 ASSI [ 5671]
   (( segid "BrD " and resid 107  and name HN  ))
   (( segid "BrD " and resid 106  and name HA  ))
      3.500      3.100      2.000 peak   5671 weight  0.11000E+01 volume  0.10620E+03 ppm1      8.981 ppm2      4.568
 ASSI [ 5681]
   (( segid "BrD " and resid 107  and name HN  ))
   (( segid "BrD " and resid 106  and name HB1 ))
      3.000      2.200      2.200 peak   5681 weight  0.11000E+01 volume  0.25814E+03 ppm1      8.980 ppm2      3.896
 ASSI [ 5691]
   (( segid "BrD " and resid 108  and name HN  ))
   (( segid "BrD " and resid 107  and name HA  ))
      3.200      2.600      2.300 peak   5691 weight  0.11000E+01 volume  0.17635E+03 ppm1      8.526 ppm2      4.447
 ASSI [ 5701]
   (( segid "BrD " and resid 108  and name HN  ))
   (( segid "BrD " and resid 107  and name HB1 ))
      2.600      1.700      1.700 peak   5701 weight  0.11000E+01 volume  0.68256E+03 ppm1      8.526 ppm2      3.671
 ASSI [ 5711]
   (( segid "BrD " and resid 109  and name HN  ))
   (( segid "BrD " and resid 108  and name HA  ))
      3.700      3.400      1.800 peak   5711 weight  0.11000E+01 volume  0.77637E+02 ppm1      8.574 ppm2      4.818
 ASSI [ 5721]
   (( segid "BrD " and resid 110  and name HN  ))
   (( segid "BrD " and resid 109  and name HA  ))
      3.700      3.400      1.800 peak   5721 weight  0.11000E+01 volume  0.78233E+02 ppm1      8.714 ppm2      4.615
 ASSI [ 5731]
   (( segid "BrD " and resid 111  and name HN  ))
   (( segid "BrD " and resid 110  and name HA  ))
      3.000      2.200      2.200 peak   5731 weight  0.11000E+01 volume  0.28368E+03 ppm1      8.168 ppm2      4.428
 ASSI [ 5741]
   (( segid "BrD " and resid 111  and name HN  ))
   (( segid "BrD " and resid 110  and name HB  ))
      2.300      1.300      1.300 peak   5741 weight  0.11000E+01 volume  0.13983E+04 ppm1      8.170 ppm2      2.353
 ASSI [ 5751]
   (( segid "BrD " and resid 111  and name HN  ))
   (( segid "BrD " and resid 112  and name HN  ))
      2.800      2.000      2.000 peak   5751 weight  0.11000E+01 volume  0.38572E+03 ppm1      8.168 ppm2      8.665
 ASSI [ 5761]
   (( segid "BrD " and resid 113  and name HN  ))
   (( segid "BrD " and resid 112  and name HA  ))
      2.700      1.800      1.800 peak   5761 weight  0.11000E+01 volume  0.46496E+03 ppm1      8.217 ppm2      4.602
 ASSI [ 5771]
   (( segid "BrD " and resid 113  and name HN  ))
   (( segid "BrD " and resid 112  and name HG1 ))
      3.800      3.600      1.700 peak   5771 weight  0.11000E+01 volume  0.63604E+02 ppm1      8.216 ppm2      2.949
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 ASSI [ 5781]
   (( segid "BrD " and resid 111  and name HN  ))
   (( segid "BrD " and resid 112  and name HG2 ))
      4.100      4.100      1.400 peak   5781 weight  0.11000E+01 volume  0.37977E+02 ppm1      8.217 ppm2      2.812
 ASSI [ 5791]
   (( segid "BrD " and resid 113  and name HN  ))
   (( segid "BrD " and resid 112  and name HB1 ))
      2.500      1.600      1.600 peak   5791 weight  0.11000E+01 volume  0.72974E+03 ppm1      8.217 ppm2      2.665
 ASSI [ 5801]
   (( segid "BrD " and resid 112  and name HN  ))
   (( segid "BrD " and resid 113  and name HN  ))
      2.500      1.600      1.600 peak   5801 weight  0.11000E+01 volume  0.81801E+03 ppm1      8.668 ppm2      8.185
 ASSI [ 5811]
   (( segid "BrD " and resid 114  and name HN  ))
   (( segid "BrD " and resid 113  and name HA  ))
      3.400      2.900      2.100 peak   5811 weight  0.11000E+01 volume  0.12247E+03 ppm1      8.376 ppm2      4.898
 ASSI [ 5821]
   (( segid "BrD " and resid 114  and name HN  ))
   (  segid "BrD " and resid 113  and name HB% )
      3.000      2.200      2.200 peak   5821 weight  0.11000E+01 volume  0.28680E+03 ppm1      8.377 ppm2      1.965
 ASSI [ 5831]
   (( segid "BrD " and resid 115  and name HN  ))
   (( segid "BrD " and resid 114  and name HA1 ))
      3.500      3.100      2.000 peak   5831 weight  0.11000E+01 volume  0.95188E+02 ppm1      8.353 ppm2      4.626
 ASSI [ 5851]
   (( segid "BrD " and resid 115  and name HN  ))
   (( segid "BrD " and resid 116  and name HN  ))
      3.700      3.400      1.800 peak   5851 weight  0.11000E+01 volume  0.76519E+02 ppm1      8.353 ppm2      8.065
 ASSI [ 5861]
   (( segid "BrD " and resid 117  and name HN  ))
   (( segid "BrD " and resid 116  and name HA  ))
      3.600      1.700      1.700 peak   5861 weight  0.11000E+01 volume  0.60302E+03 ppm1      8.884 ppm2      4.839
 ASSI [ 5871]
   (( segid "BrD " and resid 117  and name HN  ))
   (( segid "BrD " and resid 116  and name HB  ))
      3.100      2.400      2.400 peak   5871 weight  0.11000E+01 volume  0.21223E+03 ppm1      8.876 ppm2      2.417
 ASSI [ 5881]
   (( segid "BrD " and resid 118  and name HN  ))
   (( segid "BrD " and resid 117  and name HA  ))
      2.500      1.600      1.600 peak   5881 weight  0.11000E+01 volume  0.81728E+03 ppm1      8.381 ppm2      5.176
 ASSI [ 5891]
   (( segid "BrD " and resid 79   and name HE21))
   (( segid "BrD " and resid 79   and name HG1 ))
      3.900      3.800      1.600 peak   5891 weight  0.11000E+01 volume  0.58235E+02 ppm1      7.926 ppm2      3.067
 ASSI [ 5901]
   (( segid "BrD " and resid 79   and name HE22))
   (( segid "BrD " and resid 79   and name HG1 ))
      3.500      3.100      2.000 peak   5901 weight  0.11000E+01 volume  0.10842E+03 ppm1      7.829 ppm2      3.067
 ASSI [ 5911]
   (( segid "BrD " and resid 29   and name HE21))
   (( segid "BrD " and resid 29   and name HG1 ))
      4.200      4.200      1.300 peak   5911 weight  0.11000E+01 volume  0.35552E+02 ppm1      8.188 ppm2      3.028
 ASSI [ 5921]
   (( segid "BrD " and resid 29   and name HE22))
   (( segid "BrD " and resid 29   and name HG1 ))
      3.800      3.600      1.700 peak   5921 weight  0.11000E+01 volume  0.59289E+02 ppm1      7.477 ppm2      3.028
 ASSI [ 5931]
   (( segid "BrD " and resid 70   and name HN  ))
   (( segid "BrD " and resid 70   and name HB1 ))
      3.300      2.700      2.200 peak   5931 weight  0.11000E+01 volume  0.15569E+03 ppm1      8.039 ppm2      4.807
 ASSI [ 5941]
   (( segid "BrD " and resid 18   and name HN  ))
   (( segid "BrD " and resid 18   and name HB1 ))
      2.700      1.800      1.800 peak   5941 weight  0.11000E+01 volume  0.45519E+03 ppm1      9.072 ppm2      2.113
 ASSI [ 5951]
   (( segid "BrD " and resid 18   and name HN  ))
   (( segid "BrD " and resid 18   and name HG  ))
      2.600      1.700      1.700 peak   5951 weight  0.11000E+01 volume  0.60681E+03 ppm1      9.072 ppm2      2.279
 ASSI [ 5961]
   (( segid "BrD " and resid 18   and name HN  ))
   (  segid "BrD " and resid 18   and name HD2&)
      3.000      2.200      2.200 peak   5961 weight  0.11000E+01 volume  0.24628E+03 ppm1      9.076 ppm2      0.416
 ASSI [ 5971]
   (( segid "BrD " and resid 78   and name HN  ))
   (( segid "BrD " and resid 78   and name HB1 ))
      3.000      2.200      2.200 peak   5971 weight  0.11000E+01 volume  0.24153E+03 ppm1      7.996 ppm2      1.360
 ASSI [ 5981]
   (( segid "BrD " and resid 78   and name HN  ))
   (( segid "BrD " and resid 78   and name HB2 ))
      2.600      1.700      1.700 peak   5981 weight  0.11000E+01 volume  0.64225E+03 ppm1      7.996 ppm2      1.048
 ASSI [ 5991]
   (( segid "BrD " and resid 78   and name HN  ))
   (  segid "BrD " and resid 78   and name HD2&)
      3.500      3.100      2.000 peak   5991 weight  0.11000E+01 volume  0.10124E+03 ppm1      7.994 ppm2      0.667
 ASSI [ 6001]
   (( segid "BrD " and resid 78   and name HN  ))
   (( segid "BrD " and resid 78   and name HG  ))
      3.000      2.200      2.200 peak   6001 weight  0.11000E+01 volume  0.26923E+03 ppm1      7.996 ppm2      1.293
 ASSI [ 6011]
   (( segid "BrD " and resid 78   and name HN  ))
   (  segid "BrD " and resid 78   and name HD1&)
      3.500      3.100      2.000 peak   6011 weight  0.11000E+01 volume  0.10789E+03 ppm1      7.996 ppm2      0.790
 ASSI [ 6021]
   (( segid "BrD " and resid 115  and name HN  ))
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  (( segid "BrD " and resid 115  and name HB1 ))
     3.200      2.600      2.300 peak   6021 weight  0.11000E+01 volume  0.18336E+03 ppm1      8.355 ppm2      2.167
ASSI [ 6031]
  (( segid "BrD " and resid 115  and name HN ))
  ( segid "BrD " and resid 115  and name HD1%)
     2.800      2.000      2.000 peak   6031 weight  0.11000E+01 volume  0.43402E+03 ppm1      8.354 ppm2      1.318
ASSI [ 6041]
  (( segid "BrD " and resid 116  and name HN ))
  (( segid "BrD " and resid 116  and name HG11))
     2.900      2.100      2.100 peak   6041 weight  0.11000E+01 volume  0.29943E+03 ppm1      8.086 ppm2      1.921
ASSI [ 6051]
  (( segid "BrD " and resid 116  and name HN ))
  (( segid "BrD " and resid 116  and name HG12))
     3.000      2.200      2.200 peak   6051 weight  0.11000E+01 volume  0.27021E+03 ppm1      8.083 ppm2      1.525
ASSI [ 6061]
  (( segid "BrD " and resid 116  and name HN ))
  ( segid "BrD " and resid 116  and name HG2%)
     2.500      1.600      1.600 peak   6061 weight  0.11000E+01 volume  0.86711E+03 ppm1      8.084 ppm2      1.420
ASSI [ 6071]
  (( segid "BrD " and resid 110  and name HN ))
  (( segid "BrD " and resid 110  and name HG12))
     3.000      2.200      2.200 peak   6071 weight  0.11000E+01 volume  0.25527E+03 ppm1      8.714 ppm2      1.679
ASSI [ 6081]
  (( segid "BrD " and resid 110  and name HN ))
  ( segid "BrD " and resid 110  and name HG2%)
     2.800      2.000      2.000 peak   6081 weight  0.11000E+01 volume  0.43268E+03 ppm1      8.714 ppm2      1.261
ASSI [ 6091]
  (( segid "BrD " and resid 110  and name HN ))
  ( segid "BrD " and resid 110  and name HD1%)
     3.400      2.900      2.100 peak   6091 weight  0.11000E+01 volume  0.13013E+03 ppm1      8.714 ppm2      1.116
ASSI [ 6101]
  (( segid "BrD " and resid 50   and name HN ))
  (( segid "BrD " and resid 50   and name HB ))
     2.400      1.400      1.400 peak   6101 weight  0.11000E+01 volume  0.10564E+04 ppm1      8.564 ppm2      1.812
ASSI [ 6111]
  (( segid "BrD " and resid 50   and name HN ))
  ( segid "BrD " and resid 50   and name HD1%)
     3.200      2.600      2.300 peak   6111 weight  0.11000E+01 volume  0.17790E+03 ppm1      8.564 ppm2      1.144
ASSI [ 6121]
  (( segid "BrD " and resid 50   and name HN ))
  (( segid "BrD " and resid 50   and name HG12))
     3.300      2.700      2.200 peak   6121 weight  0.11000E+01 volume  0.13759E+03 ppm1      8.564 ppm2      0.823
ASSI [ 6131]
  (( segid "BrD " and resid 50   and name HN ))
  ( segid "BrD " and resid 50   and name HG2%)
     3.000      2.200      2.200 peak   6131 weight  0.11000E+01 volume  0.27674E+03 ppm1      8.564 ppm2      0.991
ASSI [ 6141]
  (( segid "BrD " and resid 50   and name HN ))
  (( segid "BrD " and resid 50   and name HG11))
     4.100      4.100      1.400 peak   6141 weight  0.11000E+01 volume  0.38065E+02 ppm1      8.564 ppm2      1.405
ASSI [ 6151]
  (( segid "BrD " and resid 21   and name HN ))
  (( segid "BrD " and resid 20   and name HB1 ))
     2.600      1.700      1.700 peak   6151 weight  0.11000E+01 volume  0.62145E+03 ppm1      8.544 ppm2      4.667
ASSI [ 6161]
  (( segid "BrD " and resid 20   and name HN ))
  (( segid "BrD " and resid 21   and name HN ))
     2.800      2.000      2.000 peak   6161 weight  0.11000E+01 volume  0.39694E+03 ppm1      8.146 ppm2      8.547
ASSI [ 6181]
  (( segid "BrD " and resid 22   and name HN ))
  (( segid "BrD " and resid 21   and name HN ))
     2.800      2.000      2.000 peak   6191 weight  0.11000E+01 volume  0.40962E+03 ppm1      9.455 ppm2      8.532
ASSI [ 6201]
  (( segid "BrD " and resid 101  and name HN ))
  (( segid "BrD " and resid 101  and name HG11))
     2.400      1.400      1.400 peak   6201 weight  0.11000E+01 volume  0.10700E+04 ppm1      8.514 ppm2      2.489
ASSI [ 6211]
  (( segid "BrD " and resid 101  and name HN ))
  (( segid "BrD " and resid 101  and name HG12))
     2.800      2.000      2.000 peak   6211 weight  0.11000E+01 volume  0.39771E+03 ppm1      8.513 ppm2      1.808
ASSI [ 6221]
  (( segid "BrD " and resid 101  and name HN ))
  ( segid "BrD " and resid 101  and name HG2%)
     2.700      1.800      1.800 peak   6221 weight  0.11000E+01 volume  0.49123E+03 ppm1      8.513 ppm2      1.596
ASSI [ 6231]
  (( segid "BrD " and resid 21   and name HN ))
  (( segid "BrD " and resid 21   and name HB ))
     2.600      1.700      1.700 peak   6231 weight  0.11000E+01 volume  0.63964E+03 ppm1      8.545 ppm2      2.495
ASSI [ 6241]
  (( segid "BrD " and resid 21   and name HN ))
  (( segid "BrD " and resid 21   and name HG11))
     2.300      1.300      1.300 peak   6241 weight  0.11000E+01 volume  0.13646E+04 ppm1      8.545 ppm2      2.355
ASSI [ 6251]
  (( segid "BrD " and resid 21   and name HN ))
  (( segid "BrD " and resid 21   and name HG12))
     3.100      2.400      2.400 peak   6251 weight  0.11000E+01 volume  0.22794E+03 ppm1      8.556 ppm2      1.659
ASSI [ 6261]
  (( segid "BrD " and resid 21   and name HN ))
  ( segid "BrD " and resid 21   and name HG2%)
     2.600      1.700      1.700 peak   6261 weight  0.11000E+01 volume  0.60538E+03 ppm1      8.556 ppm2      1.605
ASSI [ 6271]
  (( segid "BrD " and resid 21   and name HN ))
  ( segid "BrD " and resid 21   and name HD1%)
     2.900      2.100      2.100 peak   6271 weight  0.11000E+01 volume  0.30098E+03 ppm1      8.545 ppm2      1.226
ASSI [ 6281]
  (( segid "BrD " and resid 87   and name HN ))
  (( segid "BrD " and resid 87   and name HB1 ))
     2.800      2.000      2.000 peak   6281 weight  0.11000E+01 volume  0.39163E+03 ppm1      8.570 ppm2      2.771
ASSI [ 6291]
  (( segid "BrD " and resid 79   and name HN ))
  (( segid "BrD " and resid 79   and name HB1 ))
     2.500      1.600      1.600 peak   6291 weight  0.11000E+01 volume  0.73947E+03 ppm1      8.681 ppm2      2.771
ASSI [ 6301]
  (( segid "BrD " and resid 80   and name HN ))
  (( segid "BrD " and resid 79   and name HB1 ))
     2.500      2.100      2.000 peak   6301 weight  0.11000E+01 volume  0.10437E+03 ppm1      8.006 ppm2      2.764
ASSI [ 6311]
  (( segid "BrD " and resid 23   and name HN ))
  (( segid "BrD " and resid 23   and name HG2 ))
     3.200      2.600      2.300 peak   6311 weight  0.11000E+01 volume  0.19029E+03 ppm1      9.120 ppm2      3.068
ASSI [ 6321]
  (( segid "BrD " and resid 80   and name HN ))
  (( segid "BrD " and resid 80   and name HG1 ))
     3.400      2.900      2.100 peak   6321 weight  0.11000E+01 volume  0.12866E+03 ppm1      8.006 ppm2      2.336
ASSI [ 6331]
  (( segid "BrD " and resid 80   and name HN ))
  (( segid "BrD " and resid 80   and name HB1 ))
     2.800      2.000      2.000 peak   6331 weight  0.11000E+01 volume  0.38416E+03 ppm1      8.006 ppm2      2.579
ASSI [ 6341]
  (( segid "BrD " and resid 80   and name HN ))
  (( segid "BrD " and resid 80   and name HB2 ))
     2.600      1.700      1.700 peak   6341 weight  0.11000E+01 volume  0.55298E+03 ppm1      8.006 ppm2      2.497
ASSI [ 6351]
  (( segid "BrD " and resid 66   and name HN ))
  (( segid "BrD " and resid 66   and name HB2 ))
     3.400      2.900      2.100 peak   6351 weight  0.11000E+01 volume  0.12971E+03 ppm1      8.763 ppm2      2.629
ASSI [ 6361]
  (( segid "BrD " and resid 66   and name HN ))
  (( segid "BrD " and resid 66   and name HG1 ))
     2.700      1.800      1.800 peak   6361 weight  0.11000E+01 volume  0.45372E+03 ppm1      8.764 ppm2      2.155
ASSI [ 6371]
  (( segid "BrD " and resid 9    and name HN ))
  (( segid "BrD " and resid 9    and name HG1 ))
     3.600      3.200      1.900 peak   6371 weight  0.11000E+01 volume  0.84495E+02 ppm1      9.053 ppm2      2.254
ASSI [ 6381]
  (( segid "BrD " and resid 9    and name HN ))
  (( segid "BrD " and resid 9    and name HB2 ))
     3.400      2.900      2.100 peak   6381 weight  0.11000E+01 volume  0.12497E+03 ppm1      9.055 ppm2      2.369
ASSI [ 6391]
  (( segid "BrD " and resid 102  and name HN ))
  ( segid "BrD " and resid 102  and name HD1%)
     3.100      2.400      2.400 peak   6391 weight  0.11000E+01 volume  0.19704E+03 ppm1      9.156 ppm2      1.310
ASSI [ 6401]
  (( segid "BrD " and resid 102  and name HN ))
  (( segid "BrD " and resid 102  and name HB2 ))
     2.400      1.400      1.400 peak   6401 weight  0.11000E+01 volume  0.88089E+03 ppm1      9.155 ppm2      1.808
ASSI [ 6411]
  (( segid "BrD " and resid 102  and name HN ))
  (( segid "BrD " and resid 102  and name HB1 ))
     2.700      1.800      1.800 peak   6411 weight  0.11000E+01 volume  0.47200E+03 ppm1      9.155 ppm2      2.002
ASSI [ 6421]
  (( segid "BrD " and resid 102  and name HN ))
  (( segid "BrD " and resid 102  and name HG ))
     3.200      2.600      2.300 peak   6421 weight  0.11000E+01 volume  0.16630E+03 ppm1      9.157 ppm2      2.152
ASSI [ 6431]
  (( segid "BrD " and resid 73   and name HN ))
  (( segid "BrD " and resid 73   and name HB2 ))
     2.800      2.000      2.000 peak   6431 weight  0.11000E+01 volume  0.37491E+03 ppm1      8.045 ppm2      2.498
ASSI [ 6441]
  (( segid "BrD " and resid 73   and name HN ))
  (( segid "BrD " and resid 73   and name HG ))
     3.400      2.900      2.100 peak   6441 weight  0.11000E+01 volume  0.13407E+03 ppm1      8.045 ppm2      2.376
ASSI [ 6451]
  (( segid "BrD " and resid 73   and name HN ))
  ( segid "BrD " and resid 73   and name HD2%)
     3.600      3.200      1.900 peak   6451 weight  0.11000E+01 volume  0.91167E+02 ppm1      8.049 ppm2      1.491
ASSI [ 6461]
  (( segid "BrD " and resid 56   and name HN ))
  ( segid "BrD " and resid 56   and name HD1%)
     3.200      2.600      2.300 peak   6461 weight  0.11000E+01 volume  0.17282E+03 ppm1      9.679 ppm2      1.521
ASSI [ 6471]
  (( segid "BrD " and resid 56   and name HN ))
  (( segid "BrD " and resid 56   and name HG ))
     2.500      1.600      1.600 peak   6471 weight  0.11000E+01 volume  0.74688E+03 ppm1      9.680 ppm2      2.320
ASSI [ 6481]
  (( segid "BrD " and resid 56   and name HN ))
  (( segid "BrD " and resid 56   and name HB2 ))
     3.100      2.400      2.400 peak   6481 weight  0.11000E+01 volume  0.21719E+03 ppm1      9.680 ppm2      2.002
ASSI [ 6491]
  (( segid "BrD " and resid 22   and name HN ))
  ( segid "BrD " and resid 22   and name HD1%)
     3.200      2.600      2.300 peak   6491 weight  0.11000E+01 volume  0.16857E+03 ppm1      9.456 ppm2      1.668
ASSI [ 6501]
  (( segid "BrD " and resid 22   and name HN ))
  (( segid "BrD " and resid 22   and name HB2 ))
     2.400      1.400      1.400 peak   6501 weight  0.11000E+01 volume  0.10653E+04 ppm1      9.456 ppm2      2.282
ASSI [ 6511]
  (( segid "BrD " and resid 22   and name HN ))
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  (( segid "BrD " and resid 22   and name HB1 ))
     2.700     1.800     1.800 peak  6511 weight  0.11000E+01 volume  0.47530E+03 ppm1      9.455 ppm2      2.693
ASSI { 6521}
  (( segid "BrD " and resid 22   and name HN ))
  (( segid "BrD " and resid 22   and name HG ))
     3.700     3.400     1.800 peak  6521 weight  0.11000E+01 volume  0.69056E+02 ppm1      9.455 ppm2      2.366
ASSI { 6531}
  (( segid "BrD " and resid 63   and name HN ))
  (  segid "BrD " and resid 63   and name HD2%)
     3.200     2.600     2.300 peak  6531 weight  0.11000E+01 volume  0.19269E+03 ppm1      9.473 ppm2      1.478
ASSI { 6541}
  (( segid "BrD " and resid 63   and name HN ))
  (  segid "BrD " and resid 63   and name HD1%)
     3.100     2.400     2.400 peak  6541 weight  0.11000E+01 volume  0.21627E+03 ppm1      9.472 ppm2      1.674
ASSI { 6561}
  (( segid "BrD " and resid 63   and name HN ))
  (( segid "BrD " and resid 63   and name HB2 ))
     2.500     1.600     1.600 peak  6561 weight  0.11000E+01 volume  0.86099E+03 ppm1      9.473 ppm2      2.532
ASSI { 6571}
  (( segid "BrD " and resid 63   and name HN ))
  (( segid "BrD " and resid 63   and name HG ))
     3.000     2.200     2.200 peak  6571 weight  0.11000E+01 volume  0.26899E+03 ppm1      9.472 ppm2      2.439
ASSI { 6581}
  (( segid "BrD " and resid 14   and name HN ))
  (( segid "BrD " and resid 14   and name HB1 ))
     2.500     1.600     1.600 peak  6581 weight  0.11000E+01 volume  0.80229E+03 ppm1      8.809 ppm2      2.453
ASSI { 6591}
  (( segid "BrD " and resid 14   and name HN ))
  (( segid "BrD " and resid 14   and name HG ))
     3.000     2.200     2.200 peak  6591 weight  0.11000E+01 volume  0.24747E+03 ppm1      8.809 ppm2      2.064
ASSI { 6601}
  (( segid "BrD " and resid 14   and name HN ))
  (( segid "BrD " and resid 14   and name HB2 ))
     2.500     1.600     1.600 peak  6601 weight  0.11000E+01 volume  0.85081E+03 ppm1      8.809 ppm2      2.164
ASSI { 6611}
  (( segid "BrD " and resid 14   and name HN ))
  (  segid "BrD " and resid 14   and name HD1%)
     3.200     2.600     2.300 peak  6611 weight  0.11000E+01 volume  0.18673E+03 ppm1      8.809 ppm2      1.401
ASSI { 6621}
  (( segid "BrD " and resid 24   and name HN ))
  (( segid "BrD " and resid 24   and name HG2 ))
     2.300     1.300     1.300 peak  6621 weight  0.11000E+01 volume  0.12087E+04 ppm1      8.654 ppm2      3.032
ASSI { 6631}
  (( segid "BrD " and resid 49   and name HN ))
  (  segid "BrD " and resid 49   and name HG1%)
     3.100     2.400     2.400 peak  6631 weight  0.11000E+01 volume  0.20533E+03 ppm1      7.762 ppm2      1.652
ASSI { 6641}
  (( segid "BrD " and resid 50   and name HN ))
  (  segid "BrD " and resid 49   and name HG1%)
     3.400     2.900     2.100 peak  6641 weight  0.11000E+01 volume  0.12406E+03 ppm1      8.564 ppm2      1.652
ASSI { 6651}
  (( segid "BrD " and resid 64   and name HN ))
  (( segid "BrD " and resid 64   and name HB1 ))
     2.400     1.400     1.400 peak  6651 weight  0.11000E+01 volume  0.10941E+04 ppm1      8.584 ppm2      2.661
ASSI { 6661}
  (( segid "BrD " and resid 64   and name HN ))
  (( segid "BrD " and resid 64   and name HG1 ))
     2.700     1.800     1.800 peak  6661 weight  0.11000E+01 volume  0.45034E+03 ppm1      8.584 ppm2      2.210
ASSI { 6671}
  (( segid "BrD " and resid 64   and name HN ))
  (( segid "BrD " and resid 64   and name HD1 ))
     3.600     3.200     1.900 peak  6671 weight  0.11000E+01 volume  0.82950E+02 ppm1      8.584 ppm2      2.411
ASSI { 6681}
  (( segid "BrD " and resid 104  and name HN ))
  (( segid "BrD " and resid 104  and name HB1 ))
     2.600     1.700     1.700 peak  6681 weight  0.11000E+01 volume  0.59758E+03 ppm1      7.763 ppm2      2.537
ASSI { 6691}
  (( segid "BrD " and resid 104  and name HN ))
  (( segid "BrD " and resid 104  and name HG1 ))
     3.000     2.200     2.200 peak  6691 weight  0.11000E+01 volume  0.24911E+03 ppm1      7.763 ppm2      2.099
ASSI { 6701}
  (( segid "BrD " and resid 104  and name HN ))
  (( segid "BrD " and resid 104  and name HD1 ))
     2.900     2.100     2.100 peak  6701 weight  0.11000E+01 volume  0.30408E+03 ppm1      7.763 ppm2      2.288
ASSI { 6711}
  (( segid "BrD " and resid 111  and name HN ))
  (( segid "BrD " and resid 111  and name HB1 ))
     2.600     1.700     1.700 peak  6711 weight  0.11000E+01 volume  0.66813E+03 ppm1      8.168 ppm2      2.482
ASSI { 6721}
  (( segid "BrD " and resid 111  and name HN ))
  (( segid "BrD " and resid 111  and name HB2 ))
     2.400     1.400     1.400 peak  6721 weight  0.11000E+01 volume  0.98067E+03 ppm1      8.170 ppm2      2.376
ASSI { 6731}
  (( segid "BrD " and resid 111  and name HN ))
  (( segid "BrD " and resid 111  and name HG2 ))
     3.600     3.200     1.900 peak  6731 weight  0.11000E+01 volume  0.68731E+02 ppm1      8.168 ppm2      1.922
ASSI { 6741}
  (( segid "BrD " and resid 111  and name HN ))
  (( segid "BrD " and resid 111  and name HG1 ))
     3.200     2.600     2.300 peak  6741 weight  0.11000E+01 volume  0.16392E+03 ppm1      8.168 ppm2      2.002
ASSI { 6761}
  (( segid "BrD " and resid 19   and name HN ))
  (( segid "BrD " and resid 19   and name HB1 ))
     2.700     1.800     1.800 peak  6761 weight  0.11000E+01 volume  0.53478E+03 ppm1      9.187 ppm2      2.325
ASSI { 6771}
  (( segid "BrD " and resid 19   and name HN ))
  (( segid "BrD " and resid 19   and name HG1 ))
     4.000     4.000     1.500 peak  6771 weight  0.11000E+01 volume  0.45356E+02 ppm1      9.188 ppm2      1.879
ASSI { 6781}
  (( segid "BrD " and resid 19   and name HN ))
  (( segid "BrD " and resid 18   and name HG ))
     2.800     2.000     2.000 peak  6781 weight  0.11000E+01 volume  0.38486E+03 ppm1      9.187 ppm2      2.271
ASSI { 6791}
  (( segid "BrD " and resid 12   and name HN ))
  (( segid "BrD " and resid 11   and name HA ))
     3.000     2.200     2.200 peak  6791 weight  0.11000E+01 volume  0.26617E+03 ppm1      9.021 ppm2      4.940
ASSI { 6801}
  (( segid "BrD " and resid 97   and name HN ))
  (( segid "BrD " and resid 97   and name HB1 ))
     2.300     1.300     1.300 peak  6801 weight  0.11000E+01 volume  0.12859E+04 ppm1      8.674 ppm2      2.708
ASSI { 6811}
  (( segid "BrD " and resid 97   and name HN ))
  (( segid "BrD " and resid 97   and name HG2 ))
     2.900     2.100     2.100 peak  6811 weight  0.11000E+01 volume  0.32919E+03 ppm1      8.674 ppm2      2.193
ASSI { 6821}
  (( segid "BrD " and resid 109  and name HN ))
  (( segid "BrD " and resid 109  and name HB1 ))
     2.300     1.300     1.300 peak  6821 weight  0.11000E+01 volume  0.11797E+04 ppm1      8.573 ppm2      2.336
ASSI { 6831}
  (( segid "BrD " and resid 109  and name HN ))
  (( segid "BrD " and resid 109  and name HB2 ))
     3.200     2.600     2.300 peak  6831 weight  0.11000E+01 volume  0.19151E+03 ppm1      8.573 ppm2      2.173
ASSI { 6841}
  (( segid "BrD " and resid 109  and name HN ))
  (( segid "BrD " and resid 109  and name HG1 ))
     3.700     3.400     1.800 peak  6841 weight  0.11000E+01 volume  0.70793E+02 ppm1      8.574 ppm2      1.439
ASSI { 6881}
  (( segid "BrD " and resid 86   and name HN ))
  (( segid "BrD " and resid 86   and name HB1 ))
     2.700     1.800     1.800 peak  6881 weight  0.11000E+01 volume  0.51142E+03 ppm1      8.422 ppm2      2.359
ASSI { 6891}
  (( segid "BrD " and resid 86   and name HN ))
  (( segid "BrD " and resid 86   and name HG2 ))
     3.400     2.900     2.100 peak  6891 weight  0.11000E+01 volume  0.13112E+03 ppm1      8.423 ppm2      0.745
ASSI { 6901}
  (( segid "BrD " and resid 86   and name HN ))
  (( segid "BrD " and resid 86   and name HD1 ))
     3.800     3.600     1.700 peak  6901 weight  0.11000E+01 volume  0.59192E+02 ppm1      8.423 ppm2      1.862
ASSI { 6921}
  (( segid "BrD " and resid 103  and name HN ))
  (( segid "BrD " and resid 103  and name HG1 ))
     3.000     2.200     2.200 peak  6921 weight  0.11000E+01 volume  0.24153E+03 ppm1      8.695 ppm2      2.613
ASSI { 6931}
  (( segid "BrD " and resid 104  and name HN ))
  (( segid "BrD " and resid 103  and name HG1 ))
     3.200     2.600     2.300 peak  6931 weight  0.11000E+01 volume  0.18108E+03 ppm1      7.763 ppm2      2.608
ASSI { 6941}
  (( segid "BrD " and resid 48   and name HN ))
  (( segid "BrD " and resid 48   and name HG1 ))
     3.300     2.700     2.200 peak  6941 weight  0.11000E+01 volume  0.14027E+03 ppm1      8.307 ppm2      2.909
ASSI { 6951}
  (( segid "BrD " and resid 49   and name HN ))
  (( segid "BrD " and resid 48   and name HG1 ))
     4.100     4.100     1.400 peak  6951 weight  0.11000E+01 volume  0.41580E+02 ppm1      7.762 ppm2      2.932
ASSI { 6961}
  (( segid "BrD " and resid 66   and name HN ))
  (( segid "BrD " and resid 66   and name HB1 ))
     3.200     2.600     2.300 peak  6961 weight  0.11000E+01 volume  0.17814E+03 ppm1      8.763 ppm2      2.704
ASSI { 6971}
  (( segid "BrD " and resid 35   and name HN ))
  (( segid "BrD " and resid 35   and name HB1 ))
     2.900     2.100     2.100 peak  6971 weight  0.11000E+01 volume  0.32270E+03 ppm1      7.734 ppm2      2.850
ASSI { 6981}
  (( segid "BrD " and resid 54   and name HN ))
  (( segid "BrD " and resid 53   and name HA ))
     2.500     1.600     1.600 peak  6981 weight  0.11000E+01 volume  0.78564E+03 ppm1      9.036 ppm2      4.690
ASSI { 6991}
  (( segid "BrD " and resid 38   and name HN ))
  (( segid "BrD " and resid 37   and name HA ))
     2.200     1.200     1.200 peak  6991 weight  0.11000E+01 volume  0.16736E+04 ppm1      8.731 ppm2      4.849
ASSI { 7001}
  (( segid "BrD " and resid 51   and name HN ))
  (( segid "BrD " and resid 51   and name HB1 ))
     2.900     2.100     2.100 peak  7001 weight  0.11000E+01 volume  0.35413E+03 ppm1      8.375 ppm2      1.980
ASSI { 7011}
  (( segid "BrD " and resid 51   and name HN ))
  (( segid "BrD " and resid 51   and name HB2 ))
     3.000     2.200     2.200 peak  7011 weight  0.11000E+01 volume  0.24666E+03 ppm1      8.375 ppm2      1.818
ASSI { 7021}
  (( segid "BrD " and resid 51   and name HN ))
  (( segid "BrD " and resid 51   and name HG2 ))
     3.000     2.200     2.200 peak  7021 weight  0.11000E+01 volume  0.24666E+03 ppm1      8.375 ppm2      1.786
ASSI { 7041}
  (( segid "BrD " and resid 52   and name HN ))
  (( segid "BrD " and resid 52   and name HA ))
     2.900     2.100     2.100 peak  7041 weight  0.11000E+01 volume  0.32203E+03 ppm1      9.004 ppm2      5.591
ASSI { 7051}
  (( segid "BrD " and resid 52   and name HN ))
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   (( segid "BrD " and resid 52    and name HB1 ))
      2.700      1.800      1.800 peak   7051 weight  0.11000E+01 volume  0.48728E+03 ppm1      9.004 ppm2      3.641
ASSI { 7061}
   (( segid "BrD " and resid 52    and name HN  ))
   (( segid "BrD " and resid 52    and name HB2 ))
      2.500      1.600      1.600 peak   7061 weight  0.11000E+01 volume  0.72550E+03 ppm1      9.003 ppm2      3.514
ASSI { 7071}
   (( segid "BrD " and resid 52    and name HN  ))
   (( segid "BrD " and resid 51    and name HN  ))
      2.600      1.700      1.700 peak   7071 weight  0.11000E+01 volume  0.63507E+03 ppm1      9.004 ppm2      8.356
ASSI { 7091}
   (( segid "BrD " and resid 52    and name HN  ))
   (( segid "BrD " and resid 51    and name HA  ))
      3.000      2.200      2.200 peak   7091 weight  0.11000E+01 volume  0.26640E+03 ppm1      9.004 ppm2      4.482
ASSI { 7101}
   (( segid "BrD " and resid 52    and name HN  ))
   (( segid "BrD " and resid 53    and name HD1 ))
      3.500      3.100      2.000 peak   7101 weight  0.11000E+01 volume  0.10263E+03 ppm1      9.004 ppm2      4.230
ASSI { 7111}
   (( segid "BrD " and resid 52    and name HN  ))
   (( segid "BrD " and resid 53    and name HD2 ))
      3.900      3.800      1.600 peak   7111 weight  0.11000E+01 volume  0.57287E+02 ppm1      9.003 ppm2      3.997
ASSI { 7141}
   (( segid "BrD " and resid 59    and name HN  ))
   (( segid "BrD " and resid 59    and name HG2 ))
      3.300      2.700      2.200 peak   7141 weight  0.11000E+01 volume  0.14988E+03 ppm1      8.496 ppm2      1.103
ASSI { 7151}
   (( segid "BrD " and resid 59    and name HN  ))
   (( segid "BrD " and resid 59    and name HG1 ))
      3.400      2.900      2.100 peak   7151 weight  0.11000E+01 volume  0.12335E+03 ppm1      8.498 ppm2      1.228
ASSI { 7161}
   (( segid "BrD " and resid 59    and name HN  ))
   (( segid "BrD " and resid 59    and name HB1 ))
      3.400      2.900      2.100 peak   7161 weight  0.11000E+01 volume  0.11956E+03 ppm1      8.498 ppm2      2.700
ASSI { 7171}
   (( segid "BrD " and resid 59    and name HN  ))
   (( segid "BrD " and resid 59    and name HB2 ))
      3.200      2.600      2.100 peak   7171 weight  0.11000E+01 volume  0.17215E+03 ppm1      8.499 ppm2      2.504
ASSI { 7181}
   (( segid "BrD " and resid 57    and name HN  ))
   (( segid "BrD " and resid 57    and name HB1 ))
      2.400      1.400      1.400 peak   7181 weight  0.11000E+01 volume  0.94732E+03 ppm1      9.359 ppm2      2.947
ASSI { 7191}
   (( segid "BrD " and resid 57    and name HN  ))
   (( segid "BrD " and resid 57    and name HB2 ))
      2.500      1.600      1.600 peak   7191 weight  0.11000E+01 volume  0.75718E+03 ppm1      9.358 ppm2      2.827
ASSI { 7201}
   (( segid "BrD " and resid 57    and name HN  ))
   (( segid "BrD " and resid 57    and name HG1 ))
      3.600      3.200      1.900 peak   7201 weight  0.11000E+01 volume  0.93147E+02 ppm1      9.359 ppm2      2.088
ASSI { 7211}
   (( segid "BrD " and resid 57    and name HN  ))
   (( segid "BrD " and resid 57    and name HD1 ))
      4.300      4.300      1.200 peak   7211 weight  0.11000E+01 volume  0.28923E+02 ppm1      9.358 ppm2      2.411
ASSI { 7221}
   (( segid "BrD " and resid 57    and name HN  ))
   (( segid "BrD " and resid 57    and name HD2 ))
      3.400      2.900      2.100 peak   7221 weight  0.11000E+01 volume  0.13023E+03 ppm1      9.359 ppm2      2.292
ASSI { 7231}
   (( segid "BrD " and resid 26    and name HN  ))
   (( segid "BrD " and resid 26    and name HB1 ))
      3.300      2.700      2.200 peak   7231 weight  0.11000E+01 volume  0.15703E+03 ppm1      9.195 ppm2      2.463
ASSI { 7241}
   (( segid "BrD " and resid 26    and name HN  ))
   (( segid "BrD " and resid 26    and name HD1 ))
      3.500      3.100      2.000 peak   7241 weight  0.11000E+01 volume  0.99010E+02 ppm1      9.196 ppm2      2.092
ASSI { 7261}
   (( segid "BrD " and resid 10    and name HN  ))
   (( segid "BrD " and resid 11    and name HD1 ))
      4.600      4.600      0.900 peak   7261 weight  0.11000E+01 volume  0.20621E+02 ppm1      8.885 ppm2      4.475
ASSI { 7271}
   (( segid "BrD " and resid 10    and name HN  ))
   (( segid "BrD " and resid 9     and name HB1 ))
      3.400      2.900      2.100 peak   7271 weight  0.11000E+01 volume  0.12456E+03 ppm1      8.883 ppm2      2.422
ASSI { 7281}
   (( segid "BrD " and resid 13    and name HN  ))
   (( segid "BrD " and resid 12    and name HB1 ))
      3.500      3.100      2.000 peak   7281 weight  0.11000E+01 volume  0.11107E+03 ppm1      8.802 ppm2      3.399
ASSI { 7301}
   (( segid "BrD " and resid 15    and name HN  ))
   (( segid "BrD " and resid 14    and name HN  ))
      2.900      2.100      2.100 peak   7301 weight  0.11000E+01 volume  0.28689E+03 ppm1      8.597 ppm2      8.617
ASSI { 7311}
   (( segid "BrD " and resid 16    and name HN  ))
   (( segid "BrD " and resid 13    and name HA  ))
      3.500      3.100      2.000 peak   7311 weight  0.11000E+01 volume  0.96679E+02 ppm1      8.794 ppm2      4.770
ASSI { 7321}
   (( segid "BrD " and resid 15    and name HN  ))
   (  segid "BrD " and resid 14    and name HD2%)
      3.600      3.200      1.900 peak   7321 weight  0.11000E+01 volume  0.89979E+02 ppm1      8.598 ppm2      1.393
ASSI { 7331}
   (( segid "BrD " and resid 15    and name HN  ))
   (( segid "BrD " and resid 14    and name HB1 ))
      2.600      1.700      1.700 peak   7331 weight  0.11000E+01 volume  0.65160E+03 ppm1      8.599 ppm2      2.454
ASSI { 7341}
   (( segid "BrD " and resid 15    and name HN  ))
   (( segid "BrD " and resid 14    and name HB2 ))
      3.600      3.200      1.900 peak   7341 weight  0.11000E+01 volume  0.85197E+02 ppm1      8.598 ppm2      2.162
ASSI { 7351}
   (( segid "BrD " and resid 18    and name HN  ))
   (( segid "BrD " and resid 14    and name HA  ))
      3.500      3.100      2.000 peak   7351 weight  0.11000E+01 volume  0.10770E+03 ppm1      9.071 ppm2      4.652
ASSI { 7361}
   (( segid "BrD " and resid 21    and name HN  ))
   (( segid "BrD " and resid 18    and name HA  ))
      3.200      2.600      2.100 peak   7361 weight  0.11000E+01 volume  0.16933E+03 ppm1      8.544 ppm2      3.874
ASSI { 7371}
   (( segid "BrD " and resid 22    and name HN  ))
   (( segid "BrD " and resid 18    and name HA  ))
      3.700      3.400      1.800 peak   7371 weight  0.11000E+01 volume  0.72924E+02 ppm1      9.456 ppm2      3.896
ASSI { 7381}
   (( segid "BrD " and resid 19    and name HN  ))
   (( segid "BrD " and resid 16    and name HB1 ))
      2.800      2.000      2.000 peak   7381 weight  0.11000E+01 volume  0.40235E+03 ppm1      9.186 ppm2      2.139
ASSI { 7391}
   (( segid "BrD " and resid 19    and name HN  ))
   (  segid "BrD " and resid 18    and name HD1%)
      3.800      3.600      1.700 peak   7391 weight  0.11000E+01 volume  0.63600E+02 ppm1      9.189 ppm2      1.084
ASSI { 7401}
   (( segid "BrD " and resid 19    and name HN  ))
   (  segid "BrD " and resid 18    and name HD2%)
      3.700      3.400      1.800 peak   7401 weight  0.11000E+01 volume  0.71915E+02 ppm1      9.187 ppm2      0.414
ASSI { 7411}
   (( segid "BrD " and resid 20    and name HN  ))
   (( segid "BrD " and resid 19    and name HB1 ))
      3.200      2.600      2.300 peak   7411 weight  0.11000E+01 volume  0.16507E+03 ppm1      8.146 ppm2      2.336
ASSI { 7421}
   (( segid "BrD " and resid 20    and name HN  ))
   (( segid "BrD " and resid 19    and name HB2 ))
      3.400      2.900      2.100 peak   7421 weight  0.11000E+01 volume  0.13044E+03 ppm1      8.147 ppm2      1.967
ASSI { 7431}
   (( segid "BrD " and resid 23    and name HN  ))
   (( segid "BrD " and resid 19    and name HA  ))
      3.600      3.200      1.900 peak   7431 weight  0.11000E+01 volume  0.90645E+02 ppm1      9.120 ppm2      4.286
ASSI { 7441}
   (( segid "BrD " and resid 23    and name HN  ))
   (( segid "BrD " and resid 20    and name HA  ))
      3.400      2.900      2.100 peak   7441 weight  0.11000E+01 volume  0.11524E+03 ppm1      9.118 ppm2      4.895
ASSI { 7451}
   (( segid "BrD " and resid 20    and name HN  ))
   (( segid "BrD " and resid 22    and name HN  ))
      3.600      3.200      1.900 peak   7451 weight  0.11000E+01 volume  0.81392E+02 ppm1      8.147 ppm2      9.450
ASSI { 7471}
   (( segid "BrD " and resid 21    and name HN  ))
   (( segid "BrD " and resid 21    and name HN  ))
      4.100      4.100      1.400 peak   7471 weight  0.11000E+01 volume  0.42834E+02 ppm1      8.545 ppm2      9.130
ASSI { 7491}
   (( segid "BrD " and resid 24    and name HN  ))
   (( segid "BrD " and resid 21    and name HA  ))
      3.200      2.600      2.300 peak   7491 weight  0.11000E+01 volume  0.16448E+03 ppm1      8.661 ppm2      4.371
ASSI { 7501}
   (( segid "BrD " and resid 26    and name HN  ))
   (( segid "BrD " and resid 23    and name HA  ))
      3.400      2.900      2.100 peak   7501 weight  0.11000E+01 volume  0.12059E+03 ppm1      9.196 ppm2      4.639
ASSI { 7511}
   (( segid "BrD " and resid 27    and name HN  ))
   (( segid "BrD " and resid 24    and name HA  ))
      3.200      2.600      2.300 peak   7511 weight  0.11000E+01 volume  0.17746E+03 ppm1      8.170 ppm2      4.777
ASSI { 7521}
   (( segid "BrD " and resid 28    and name HN  ))
   (( segid "BrD " and resid 25    and name HA  ))
      3.600      3.200      1.900 peak   7521 weight  0.11000E+01 volume  0.92661E+02 ppm1      8.166 ppm2      4.449
ASSI { 7531}
   (( segid "BrD " and resid 26    and name HN  ))
   (( segid "BrD " and resid 25    and name HB  ))
      2.600      1.700      1.700 peak   7531 weight  0.11000E+01 volume  0.67212E+03 ppm1      9.196 ppm2      2.991
ASSI { 7541}
   (( segid "BrD " and resid 26    and name HN  ))
   (  segid "BrD " and resid 25    and name HG2%)
      2.900      2.100      2.100 peak   7541 weight  0.11000E+01 volume  0.31151E+03 ppm1      9.196 ppm2      1.640
ASSI { 7551}
   (( segid "BrD " and resid 26    and name HN  ))
   (  segid "BrD " and resid 25    and name HG1%)
      3.100      2.400      2.400 peak   7551 weight  0.11000E+01 volume  0.21302E+03 ppm1      9.197 ppm2      1.790
ASSI { 7561}
   (( segid "BrD " and resid 43    and name HN  ))
   (( segid "BrD " and resid 44    and name HD1 ))
      3.400      2.900      2.100 peak   7561 weight  0.11000E+01 volume  0.11281E+03 ppm1      8.001 ppm2      4.324
ASSI { 7571}
   (( segid "BrD " and resid 43    and name HN  ))
   (( segid "BrD " and resid 44    and name HD2 ))
      3.100      2.400      2.400 peak   7571 weight  0.11000E+01 volume  0.21754E+03 ppm1      8.001 ppm2      6.122
ASSI { 7581}
   (( segid "BrD " and resid 49    and name HN  ))
   (( segid "BrD " and resid 46    and name HA  ))
      3.900      3.800      1.600 peak   7581 weight  0.11000E+01 volume  0.54216E+02 ppm1      7.763 ppm2      4.143
ASSI { 7591}
   (( segid "BrD " and resid 56    and name HN  ))
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   (( segid "BrD " and resid 56   and name HB1 ))
      2.700     1.800     1.800 peak  7591 weight  0.11000E+01 volume  0.48254E+03 ppm1      9.679 ppm2      2.693
ASSI { 7601}
   (( segid "BrD " and resid 61   and name HN  ))
   (( segid "BrD " and resid 58   and name HA  ))
      2.900     2.100     2.100 peak  7601 weight  0.11000E+01 volume  0.30089E+03 ppm1      8.749 ppm2      4.452
ASSI { 7611}
   (( segid "BrD " and resid 64   and name HN  ))
   (( segid "BrD " and resid 60   and name HA  ))
      3.400     2.900     2.100 peak  7611 weight  0.11000E+01 volume  0.11932E+03 ppm1      8.584 ppm2      4.807
ASSI { 7621}
   (( segid "BrD " and resid 66   and name HN  ))
   (( segid "BrD " and resid 66   and name HD1 ))
      2.900     2.100     2.100 peak  7621 weight  0.11000E+01 volume  0.29994E+01 ppm1      8.759 ppm2      3.667
ASSI { 7631}
   (( segid "BrD " and resid 75   and name HN  ))
   (( segid "BrD " and resid 72   and name HA  ))
      3.400     2.900     2.100 peak  7631 weight  0.11000E+01 volume  0.13400E+03 ppm1      9.106 ppm2      4.669
ASSI { 7651}
   (( segid "BrD " and resid 79   and name HN  ))
   (( segid "BrD " and resid 76   and name HA  ))
      3.200     2.600     2.300 peak  7651 weight  0.11000E+01 volume  0.16410E+03 ppm1      8.680 ppm2      4.691
ASSI { 7661}
   (( segid "BrD " and resid 80   and name HN  ))
   (( segid "BrD " and resid 77   and name HA  ))
      3.700     3.400     1.800 peak  7661 weight  0.11000E+01 volume  0.79484E+02 ppm1      8.006 ppm2      4.969
ASSI { 7671}
   (( segid "BrD " and resid 81   and name HN  ))
   (( segid "BrD " and resid 78   and name HA  ))
      3.200     2.700     2.200 peak  7671 weight  0.11000E+01 volume  0.15049E+03 ppm1      7.639 ppm2      3.989
ASSI { 7681}
   (( segid "BrD " and resid 82   and name HN  ))
   (( segid "BrD " and resid 79   and name HA  ))
      3.600     3.200     1.900 peak  7681 weight  0.11000E+01 volume  0.80779E+02 ppm1      6.981 ppm2      4.411
ASSI { 7701}
   (( segid "BrD " and resid 84   and name HN  ))
   (( segid "BrD " and resid 81   and name HA  ))
      3.500     3.100     2.000 peak  7701 weight  0.11000E+01 volume  0.10576E+03 ppm1      9.463 ppm2      3.705
ASSI { 7711}
   (( segid "BrD " and resid 85   and name HN  ))
   (( segid "BrD " and resid 82   and name HA  ))
      3.300     2.700     2.200 peak  7711 weight  0.11000E+01 volume  0.13652E+03 ppm1      7.516 ppm2      4.768
ASSI { 7721}
   (( segid "BrD " and resid 89   and name HN  ))
   (( segid "BrD " and resid 86   and name HA  ))
      3.500     3.100     2.000 peak  7721 weight  0.11000E+01 volume  0.10495E+03 ppm1      8.858 ppm2      4.811
ASSI { 7731}
   (( segid "BrD " and resid 93   and name HN  ))
   (( segid "BrD " and resid 92   and name HA  ))
      3.600     3.200     1.900 peak  7731 weight  0.11000E+01 volume  0.94491E+02 ppm1      8.713 ppm2      4.796
ASSI { 7741}
   (( segid "BrD " and resid 98   and name HN  ))
   (( segid "BrD " and resid 95   and name HA  ))
      3.300     2.700     2.200 peak  7741 weight  0.11000E+01 volume  0.14245E+03 ppm1      9.125 ppm2      4.441
ASSI { 7751}
   (( segid "BrD " and resid 77   and name HN  ))
   (( segid "BrD " and resid 75   and name HN  ))
      3.500     3.100     2.000 peak  7751 weight  0.11000E+01 volume  0.10255E+03 ppm1      7.985 ppm2      9.096
ASSI { 7761}
   (( segid "BrD " and resid 98   and name HN  ))
   (( segid "BrD " and resid 96   and name HN  ))
      3.900     3.800     1.600 peak  7761 weight  0.11000E+01 volume  0.51137E+02 ppm1      9.125 ppm2      7.963
ASSI { 7771}
   (( segid "BrD " and resid 102  and name HN  ))
   (( segid "BrD " and resid 98   and name HA  ))
      3.500     3.100     2.000 peak  7771 weight  0.11000E+01 volume  0.10795E+03 ppm1      9.156 ppm2      4.809
ASSI { 7781}
   (( segid "BrD " and resid 102  and name HN  ))
   (( segid "BrD " and resid 99   and name HA  ))
      3.500     3.100     2.000 peak  7781 weight  0.11000E+01 volume  0.10223E+03 ppm1      9.156 ppm2      4.443
ASSI { 7791}
   (( segid "BrD " and resid 103  and name HN  ))
   (( segid "BrD " and resid 100  and name HA  ))
      3.000     2.200     2.200 peak  7791 weight  0.11000E+01 volume  0.26822E+03 ppm1      8.696 ppm2      4.932
ASSI { 7801}
   (( segid "BrD " and resid 104  and name HN  ))
   (( segid "BrD " and resid 101  and name HA  ))
      3.000     2.200     2.200 peak  7801 weight  0.11000E+01 volume  0.25521E+03 ppm1      7.763 ppm2      4.275
ASSI { 7811}
   (( segid "BrD " and resid 102  and name HN  ))
   (( segid "BrD " and resid 104  and name HN  ))
      4.300     4.300     1.200 peak  7811 weight  0.11000E+01 volume  0.28976E+02 ppm1      9.156 ppm2      7.772
ASSI { 7831}
   (( segid "BrD " and resid 105  and name HN  ))
   (( segid "BrD " and resid 102  and name HA  ))
      3.300     2.700     2.200 peak  7831 weight  0.11000E+01 volume  0.14640E+03 ppm1      8.488 ppm2      4.290
ASSI { 7841}
   (( segid "BrD " and resid 108  and name HN  ))
   (( segid "BrD " and resid 105  and name HA  ))
      3.600     3.200     1.900 peak  7841 weight  0.11000E+01 volume  0.82783E+02 ppm1      8.526 ppm2      4.936
ASSI { 7851}
   (( segid "BrD " and resid 16   and name HN  ))
   (( segid "BrD " and resid 16   and name HB1 ))
      2.900     2.100     2.100 peak  7851 weight  0.11000E+01 volume  0.35014E+03 ppm1      8.794 ppm2      4.587
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ASSI { 7861}
   (( segid "BrD " and resid 24   and name HE22))
   (( segid "BrD " and resid 24   and name HG2 ))
      4.100     4.100     1.400 peak  7861 weight  0.11000E+01 volume  0.40620E+02 ppm1      7.523 ppm2      3.068
ASSI { 7871}
   (( segid "BrD " and resid 24   and name HE21))
   (( segid "BrD " and resid 24   and name HG2 ))
      3.500     3.100     2.000 peak  7871 weight  0.11000E+01 volume  0.10084E+03 ppm1      7.629 ppm2      3.067
ASSI { 7881}
   (( segid "BrD " and resid 25   and name HN  ))
   (( segid "BrD " and resid 24   and name HG1 ))
      3.400     2.900     3.100 peak  7881 weight  0.11000E+01 volume  0.11666E+03 ppm1      9.133 ppm2      3.447
ASSI { 7891}
   (( segid "BrD " and resid 18   and name HN  ))
   (  segid "BrD " and resid 18   and name HD1%)
      2.900     2.100     2.100 peak  7891 weight  0.11000E+01 volume  0.29964E+03 ppm1      9.072 ppm2      1.068
ASSI { 7901}
   (( segid "BrD " and resid 73   and name HN  ))
   (  segid "BrD " and resid 73   and name HD1%)
      3.300     2.700     2.200 peak  7901 weight  0.11000E+01 volume  0.15507E+03 ppm1      8.049 ppm2      1.540
ASSI { 7911}
   (( segid "BrD " and resid 73   and name HN  ))
   (( segid "BrD " and resid 73   and name HB1 ))
      2.800     2.000     2.000 peak  7911 weight  0.11000E+01 volume  0.38621E+03 ppm1      8.045 ppm2      2.590
ASSI { 7921}
   (( segid "BrD " and resid 56   and name HN  ))
   (  segid "BrD " and resid 56   and name HD2%)
      3.100     2.400     2.400 peak  7921 weight  0.11000E+01 volume  0.19974E+03 ppm1      9.679 ppm2      1.235
ASSI { 7931}
   (( segid "BrD " and resid 22   and name HN  ))
   (  segid "BrD " and resid 22   and name HD2%)
      3.000     2.200     2.200 peak  7931 weight  0.11000E+01 volume  0.25836E+03 ppm1      9.455 ppm2      1.584
ASSI { 7941}
   (( segid "BrD " and resid 110  and name HN  ))
   (( segid "BrD " and resid 110  and name HG11))
      2.900     2.100     2.100 peak  7941 weight  0.11000E+01 volume  0.31947E+03 ppm1      8.715 ppm2      1.745
ASSI { 7951}
   (( segid "BrD " and resid 29   and name HN  ))
   (( segid "BrD " and resid 29   and name HG1 ))
      3.100     2.400     2.400 peak  7951 weight  0.11000E+01 volume  0.23530E+03 ppm1      9.152 ppm2      3.021
ASSI { 7961}
   (( segid "BrD " and resid 23   and name HN  ))
   (( segid "BrD " and resid 23   and name HB2 ))
      2.400     1.400     1.400 peak  7961 weight  0.11000E+01 volume  0.91388E+03 ppm1      9.120 ppm2      2.851
ASSI { 7971}
   (( segid "BrD " and resid 80   and name HN  ))
   (( segid "BrD " and resid 80   and name HD2 ))
      4.400     4.400     1.100 peak  7971 weight  0.11000E+01 volume  0.24560E+02 ppm1      8.007 ppm2      3.932
ASSI { 7981}
   (( segid "BrD " and resid 100  and name HN  ))
   (( segid "BrD " and resid 100  and name HB1 ))
      2.800     2.000     2.000 peak  7981 weight  0.11000E+01 volume  0.39419E+03 ppm1      8.669 ppm2      3.493
ASSI { 7991}
   (( segid "BrD " and resid 19   and name HN  ))
   (( segid "BrD " and resid 19   and name HB2 ))
      3.000     2.200     2.200 peak  7991 weight  0.11000E+01 volume  0.28394E+03 ppm1      9.187 ppm2      1.971
ASSI { 8001}
   (( segid "BrD " and resid 97   and name HN  ))
   (( segid "BrD " and resid 97   and name HG1 ))
      2.500     1.600     1.600 peak  8001 weight  0.11000E+01 volume  0.82725E+03 ppm1      8.674 ppm2      2.415
ASSI { 8011}
   (( segid "BrD " and resid 105  and name HN  ))
   (( segid "BrD " and resid 105  and name HB2 ))
      3.100     2.400     2.400 peak  8011 weight  0.11000E+01 volume  0.23309E+03 ppm1      8.487 ppm2      3.654
ASSI { 8021}
   (( segid "BrD " and resid 12   and name HN  ))
   (( segid "BrD " and resid 12   and name HB2 ))
      3.100     2.400     2.400 peak  8021 weight  0.11000E+01 volume  0.23285E+03 ppm1      9.021 ppm2      3.337
ASSI { 8031}
   (( segid "BrD " and resid 10   and name HN  ))
   (( segid "BrD " and resid 10   and name HB2 ))
      3.000     2.200     2.200 peak  8031 weight  0.11000E+01 volume  0.26676E+03 ppm1      8.886 ppm2      3.299
ASSI { 8041}
   (( segid "BrD " and resid 114  and name HN  ))
   (( segid "BrD " and resid 114  and name HA2 ))
      2.800     2.000     2.000 peak  8041 weight  0.11000E+01 volume  0.43716E+03 ppm1      8.375 ppm2      4.531
ASSI { 8051}
   (( segid "BrD " and resid 85   and name HN  ))
   (( segid "BrD " and resid 85   and name HB2 ))
      3.100     2.400     2.400 peak  8051 weight  0.11000E+01 volume  0.21741E+03 ppm1      7.517 ppm2      3.603
ASSI { 8101}
   (( segid "BrD " and resid 39   and name HN  ))
   (( segid "BrD " and resid 39   and name HB1 ))
      2.800     2.000     2.000 peak  8101 weight  0.11000E+01 volume  0.36178E+03 ppm1      9.651 ppm2      2.480
ASSI { 8111}
   (( segid "BrD " and resid 39   and name HN  ))
   (( segid "BrD " and resid 39   and name HD1 ))
      2.500     1.600     1.600 peak  8111 weight  0.11000E+01 volume  0.74538E+03 ppm1      9.653 ppm2      2.280
ASSI { 8121}
   (( segid "BrD " and resid 39   and name HN  ))
   (( segid "BrD " and resid 39   and name HG1 ))
      3.100     2.400     2.400 peak  8121 weight  0.11000E+01 volume  0.20991E+03 ppm1      9.651 ppm2      2.042
ASSI { 8131}
   (( segid "BrD " and resid 57   and name HN  ))
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   (( segid "BrD " and resid 59   and name HN  ))
      3.700     3.400     1.800 peak  8131 weight  0.11000E+01 volume  0.75860E+02 ppm1      9.355 ppm2      8.478
ASSI { 8171}
   (( segid "BrD " and resid 57   and name HN  ))
   (( segid "BrD " and resid 56   and name HB1 ))
      2.800     2.000     2.000 peak  8171 weight  0.11000E+01 volume  0.40297E+03 ppm1      9.359 ppm2      2.702
ASSI { 8191}
   (( segid "BrD " and resid 57   and name HN  ))
    ( segid "BrD " and resid 56   and name HD1%)
      3.700     3.400     1.800 peak  8191 weight  0.11000E+01 volume  0.68904E+02 ppm1      9.358 ppm2      1.547
ASSI { 8201}
   (( segid "BrD " and resid 57   and name HN  ))
   (( segid "BrD " and resid 57   and name HG2 ))
      3.700     3.400     1.800 peak  8201 weight  0.11000E+01 volume  0.72644E+02 ppm1      9.361 ppm2      2.011
ASSI { 8241}
   (( segid "BrD " and resid 28   and name HN  ))
   (( segid "BrD " and resid 24   and name HA  ))
      3.600     3.200     1.900 peak  8241 weight  0.11000E+01 volume  0.82533E+02 ppm1      8.166 ppm2      4.803
ASSI { 8251}
   (( segid "BrD " and resid 28   and name HN  ))
   (( segid "BrD " and resid 28   and name HD2 ))
      3.800     3.600     1.700 peak  8251 weight  0.11000E+01 volume  0.64220E+02 ppm1      8.166 ppm2      5.585
ASSI { 8351}
   (( segid "BrD " and resid 51   and name HN  ))
    ( segid "BrD " and resid 50   and name HG2%)
      3.000     2.200     2.200 peak  8351 weight  0.11000E+01 volume  0.27507E+03 ppm1      8.379 ppm2      0.982
ASSI { 8431}
   (( segid "BrD " and resid 117  and name HN  ))
    ( segid "BrD " and resid 116  and name HG2%)
      3.700     3.400     1.800 peak  8431 weight  0.11000E+01 volume  0.73143E+02 ppm1      8.677 ppm2      1.422
ASSI { 8471}
   (( segid "BrD " and resid 102  and name HN  ))
   (( segid "BrD " and resid 101  and name HB  ))
      3.000     2.200     2.200 peak  8471 weight  0.11000E+01 volume  0.25477E+03 ppm1      9.156 ppm2      2.531
ASSI { 8491}
   (( segid "BrD " and resid 102  and name HN  ))
    ( segid "BrD " and resid 101  and name HG2%)
      3.300     2.700     2.200 peak  8491 weight  0.11000E+01 volume  0.14766E+03 ppm1      9.156 ppm2      1.598
ASSI { 8541}
   (( segid "BrD " and resid 46   and name HN  ))
    ( segid "BrD " and resid 46   and name HD% )
      3.500     3.100     2.000 peak  8541 weight  0.11000E+01 volume  0.10722E+03 ppm1      8.562 ppm2      5.719
ASSI { 8591}
   (( segid "BrD " and resid 43   and name HN  ))
   (( segid "BrD " and resid 41   and name HA  ))
      3.000     2.200     2.200 peak  8591 weight  0.11000E+01 volume  0.24489E+03 ppm1      8.001 ppm2      4.645
ASSI { 8671}
   (( segid "BrD " and resid 111  and name HN  ))
   (( segid "BrD " and resid 110  and name HG11)),
      3.600     3.200     1.900 peak  8671 weight  0.11000E+01 volume  0.81338E+02 ppm1      8.168 ppm2      1.747
ASSI { 8701}
   (( segid "BrD " and resid 111  and name HN  ))
    ( segid "BrD " and resid 110  and name HD1%)
      4.000     4.000     1.500 peak  8701 weight  0.11000E+01 volume  0.48240E+02 ppm1      8.168 ppm2      1.148
ASSI { 8731}
   (( segid "BrD " and resid 58   and name HN  ))
   (( segid "BrD " and resid 57   and name HB1 ))
      3.100     2.400     2.400 peak  8731 weight  0.11000E+01 volume  0.22478E+03 ppm1     10.051 ppm2      2.937
ASSI { 8741}
   (( segid "BrD " and resid 58   and name HN  ))
   (( segid "BrD " and resid 57   and name HB2 ))
      3.100     2.400     2.400 peak  8741 weight  0.11000E+01 volume  0.21458E+03 ppm1     10.051 ppm2      2.831
ASSI { 8761}
   (( segid "BrD " and resid 58   and name HN  ))
   (( segid "BrD " and resid 57   and name HD1 ))
      4.300     4.300     1.200 peak  8761 weight  0.11000E+01 volume  0.29553E+02 ppm1     10.051 ppm2      2.400
ASSI { 8771}
   (( segid "BrD " and resid 58   and name HN  ))
   (( segid "BrD " and resid 57   and name HD2 ))
      3.800     3.600     1.700 peak  8771 weight  0.11000E+01 volume  0.60769E+02 ppm1     10.051 ppm2      2.303
ASSI { 8781}
   (( segid "BrD " and resid 58   and name HN  ))
   (( segid "BrD " and resid 57   and name HG1 ))
      3.800     3.600     1.700 peak  8781 weight  0.11000E+01 volume  0.60094E+02 ppm1     10.051 ppm2      2.090
ASSI { 8791}
   (( segid "BrD " and resid 58   and name HN  ))
   (( segid "BrD " and resid 57   and name HG2 ))
      3.800     3.600     1.700 peak  8791 weight  0.11000E+01 volume  0.67776E+02 ppm1     10.051 ppm2      2.010
ASSI { 8821}
   (( segid "BrD " and resid 10   and name HN  ))
   (( segid "BrD " and resid 9    and name HG1 ))
      4.100     4.100     1.400 peak  8821 weight  0.11000E+01 volume  0.38664E+02 ppm1      8.885 ppm2      2.288
ASSI { 8831}
   (( segid "BrD " and resid 13   and name HN  ))
   (( segid "BrD " and resid 12   and name HB2 ))
      3.400     2.900     2.100 peak  8831 weight  0.11000E+01 volume  0.11575E+03 ppm1      8.803 ppm2      3.337
ASSI { 8841}
   (( segid "BrD " and resid 14   and name HN  ))
   (( segid "BrD " and resid 12   and name HN  ))
      2.600     1.700     1.700 peak  8841 weight  0.11000E+01 volume  0.56119E+03 ppm1      8.803 ppm2      9.004
ASSI { 8921}
   (( segid "BrD " and resid 112  and name HN  ))
   (( segid "BrD " and resid 111  and name HB1 ))
      2.700     1.800     1.800 peak  8921 weight  0.11000E+01 volume  0.53559E+03 ppm1      8.666 ppm2      2.473
ASSI { 8931}
   (( segid "BrD " and resid 112  and name HN  ))
   (( segid "BrD " and resid 111  and name HB2 ))
      3.100     2.400     2.400 peak  8931 weight  0.11000E+01 volume  0.20903E+03 ppm1      8.667 ppm2      2.363
ASSI { 8951}
   (( segid "BrD " and resid 112  and name HN  ))
   (( segid "BrD " and resid 111  and name HG1 ))
      3.800     3.600     1.700 peak  8951 weight  0.11000E+01 volume  0.66936E+02 ppm1      8.666 ppm2      1.997
ASSI { 9001}
   (( segid "BrD " and resid 105  and name HN  ))
   (( segid "BrD " and resid 104  and name HB1 ))
      2.600     1.700     1.700 peak  9001 weight  0.11000E+01 volume  0.67760E+03 ppm1      8.487 ppm2      2.536
ASSI { 9021}
   (( segid "BrD " and resid 105  and name HN  ))
   (( segid "BrD " and resid 104  and name HG1 ))
      4.800     4.800     0.700 peak  9021 weight  0.11000E+01 volume  0.16288E+02 ppm1      8.485 ppm2      2.099
ASSI { 9081}
   (( segid "BrD " and resid 109  and name HN  ))
   (( segid "BrD " and resid 108  and name HB1 ))
      2.500     1.600     1.600 peak  9081 weight  0.11000E+01 volume  0.75253E+03 ppm1      8.573 ppm2      4.614
ASSI { 9141}
   (( segid "BrD " and resid 106  and name HN  ))
    ( segid "BrD " and resid 106  and name HD% )
      3.700     3.400     1.800 peak  9141 weight  0.11000E+01 volume  0.76595E+02 ppm1      9.740 ppm2      7.511
ASSI { 9151}
   (( segid "BrD " and resid 106  and name HN  ))
   (( segid "BrD " and resid 102  and name HA  ))
      3.700     3.400     1.800 peak  9151 weight  0.11000E+01 volume  0.78592E+02 ppm1      9.740 ppm2      4.277
ASSI { 9301}
   (( segid "BrD " and resid 63   and name HN  ))
   (( segid "BrD " and resid 60   and name HA  ))
      3.800     3.600     1.700 peak  9301 weight  0.11000E+01 volume  0.67510E+02 ppm1      9.471 ppm2      4.809
ASSI { 9321}
   (( segid "BrD " and resid 63   and name HN  ))
   (( segid "BrD " and resid 62   and name HB1 ))
      2.200     1.200     1.200 peak  9321 weight  0.11000E+01 volume  0.14701E+04 ppm1      9.472 ppm2      2.654
ASSI { 9331}
   (( segid "BrD " and resid 63   and name HN  ))
   (( segid "BrD " and resid 61   and name HN  ))
      3.500     3.100     2.000 peak  9331 weight  0.11000E+01 volume  0.10977E+03 ppm1      9.475 ppm2      8.757
ASSI { 9351}
   (( segid "BrD " and resid 22   and name HN  ))
   (( segid "BrD " and resid 20   and name HA  ))
      4.100     4.100     1.400 peak  9351 weight  0.11000E+01 volume  0.39214E+02 ppm1      9.458 ppm2      4.872
ASSI { 9361}
   (( segid "BrD " and resid 22   and name HN  ))
   (( segid "BrD " and resid 19   and name HA  ))
      3.600     3.200     1.900 peak  9361 weight  0.11000E+01 volume  0.85958E+02 ppm1      9.457 ppm2      4.286
ASSI { 9391}
   (( segid "BrD " and resid 22   and name HN  ))
   (( segid "BrD " and resid 21   and name HB  ))
      2.700     1.800     1.800 peak  9391 weight  0.11000E+01 volume  0.51430E+03 ppm1      9.457 ppm2      2.491
ASSI { 9551}
   (( segid "BrD " and resid 103  and name HN  ))
   (( segid "BrD " and resid 99   and name HA  ))
      4.600     4.600     0.900 peak  9551 weight  0.11000E+01 volume  0.21373E+02 ppm1      8.695 ppm2      4.441
ASSI { 9571}
   (( segid "BrD " and resid 103  and name HN  ))
   (( segid "BrD " and resid 102  and name HG  ))
      3.200     2.600     2.300 peak  9571 weight  0.11000E+01 volume  0.17364E+03 ppm1      8.695 ppm2      2.187
ASSI { 9581}
   (( segid "BrD " and resid 103  and name HN  ))
    ( segid "BrD " and resid 101  and name HG2%)
      3.000     2.200     2.200 peak  9581 weight  0.11000E+01 volume  0.23656E+03 ppm1      8.695 ppm2      1.624
ASSI { 9591}
   (( segid "BrD " and resid 103  and name HN  ))
    ( segid "BrD " and resid 102  and name HD1%)
      3.600     3.200     1.900 peak  9591 weight  0.11000E+01 volume  0.85679E+02 ppm1      8.695 ppm2      1.308
ASSI { 9601}
   (( segid "BrD " and resid 103  and name HN  ))
   (( segid "BrD " and resid 102  and name HB2 ))
      3.200     2.600     2.300 peak  9601 weight  0.11000E+01 volume  0.18049E+03 ppm1      8.695 ppm2      1.806
ASSI { 9691}
   (( segid "BrD " and resid 18   and name HN  ))
   (( segid "BrD " and resid 18   and name HB2 ))
      2.800     2.000     2.000 peak  9691 weight  0.11000E+01 volume  0.37426E+03 ppm1      9.073 ppm2      0.909
ASSI { 9701}
   (( segid "BrD " and resid 64   and name HN  ))
   (( segid "BrD " and resid 61   and name HA  ))
      3.100     2.400     2.400 peak  9701 weight  0.11000E+01 volume  0.22483E+03 ppm1      8.584 ppm2      4.652
ASSI { 9711}
   (( segid "BrD " and resid 64   and name HN  ))
   (( segid "BrD " and resid 62   and name HA  ))
      3.900     3.800     1.600 peak  9711 weight  0.11000E+01 volume  0.56508E+02 ppm1      8.583 ppm2      4.488
ASSI { 9741}
   (( segid "BrD " and resid 64   and name HN  ))
   (( segid "BrD " and resid 63   and name HB1 ))
      2.600     1.700     1.700 peak  9741 weight  0.11000E+01 volume  0.57592E+03 ppm1      8.585 ppm2      2.902
ASSI { 9931}
   (( segid "BrD " and resid 62   and name HN  ))
   (( segid "BrD " and resid 62   and name HB2 ))
      2.900     2.100     2.100 peak  9931 weight  0.11000E+01 volume  0.30063E+03 ppm1      8.998 ppm2      1.683
ASSI { 9941}
   (( segid "BrD " and resid 62   and name HN  ))
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   (( segid "BrD " and resid 62   and name HG2 ))
     3.700     3.400     1.800 peak  9941 weight  0.11000E+01 volume  0.71463E+02 ppm1      8.998 ppm2      1.484
ASSI ( 9961)
   (( segid "BrD " and resid 12   and name HN  ))
   (( segid "BrD " and resid 11   and name HD1 ))
     2.800     2.000     2.000 peak  9961 weight  0.11000E+01 volume  0.35721E+03 ppm1      9.021 ppm2      4.473
ASSI (10011)
   (( segid "BrD " and resid 25   and name HN  ))
   (( segid "BrD " and resid 22   and name HA  ))
     3.300     2.700     2.200 peak 10011 weight  0.11000E+01 volume  0.14084E+03 ppm1      9.133 ppm2      4.697
ASSI (10041)
   (( segid "BrD " and resid 24   and name HN  ))
   (( segid "BrD " and resid 23   and name HB1 ))
     2.600     1.700     1.700 peak 10041 weight  0.11000E+01 volume  0.58902E+03 ppm1      8.655 ppm2      2.934
ASSI (10051)
   (( segid "BrD " and resid 24   and name HN  ))
   (  segid "BrD " and resid 21   and name HG2%)
     3.600     3.200     1.900 peak 10051 weight  0.11000E+01 volume  0.85488E+02 ppm1      8.656 ppm2      1.610
ASSI (10071)
   (( segid "BrD " and resid 24   and name HN  ))
   (( segid "BrD " and resid 20   and name HA  ))
     3.800     3.600     1.700 peak 10071 weight  0.11000E+01 volume  0.60003E+02 ppm1      8.659 ppm2      4.888
ASSI (10101)
   (( segid "BrD " and resid 15   and name HN  ))
   (( segid "BrD " and resid 13   and name HB1 ))
     3.500     3.100     2.000 peak 10101 weight  0.11000E+01 volume  0.10487E+03 ppm1      8.599 ppm2      2.755
ASSI (10161)
   (( segid "BrD " and resid 16   and name HN  ))
   (( segid "BrD " and resid 15   and name HA  ))
     2.800     2.000     2.000 peak 10161 weight  0.11000E+01 volume  0.35770E+03 ppm1      8.796 ppm2      4.617
ASSI (10171)
   (( segid "BrD " and resid 16   and name HN  ))
   (  segid "BrD " and resid 15   and name HD% )
     3.500     3.100     2.000 peak 10171 weight  0.11000E+01 volume  0.11249E+03 ppm1      8.792 ppm2      7.660
ASSI (10211)
   (( segid "BrD " and resid 75   and name HN  ))
   (( segid "BrD " and resid 73   and name HA  ))
     3.900     3.800     1.600 peak 10211 weight  0.11000E+01 volume  0.50909E+02 ppm1      9.106 ppm2      4.820
ASSI (10271)
   (( segid "BrD " and resid 75   and name HN  ))
   (  segid "BrD " and resid 74   and name HD% )
     3.200     2.600     2.300 peak 10271 weight  0.11000E+01 volume  0.18529E+03 ppm1      9.107 ppm2      7.007
ASSI (10321)
   (( segid "BrD " and resid 96   and name HN  ))
   (( segid "BrD " and resid 95   and name HB2 ))
     2.600     1.700     1.700 peak 10321 weight  0.11000E+01 volume  0.63650E+03 ppm1      7.979 ppm2      3.345
ASSI (10341)
   (( segid "BrD " and resid 95   and name HN  ))
   (( segid "BrD " and resid 92   and name HA  ))
     3.400     2.900     2.100 peak 10341 weight  0.11000E+01 volume  0.12625E+03 ppm1      8.669 ppm2      4.792
ASSI (10361)
   (( segid "BrD " and resid 95   and name HN  ))
   (  segid "BrD " and resid 95   and name HD% )
     3.400     2.900     2.100 peak 10361 weight  0.11000E+01 volume  0.13077E+03 ppm1      8.670 ppm2      7.500
ASSI (10371)
   (( segid "BrD " and resid 96   and name HN  ))
   (  segid "BrD " and resid 96   and name HD% )
     3.300     2.700     2.200 peak 10371 weight  0.11000E+01 volume  0.14891E+03 ppm1      7.979 ppm2      7.701
ASSI (10481)
   (( segid "BrD " and resid 78   and name HN  ))
   (( segid "BrD " and resid 75   and name HA  ))
     3.100     2.400     2.400 peak 10481 weight  0.11000E+01 volume  0.20590E+03 ppm1      7.996 ppm2      4.532
ASSI (10491)
   (( segid "BrD " and resid 78   and name HN  ))
   (( segid "BrD " and resid 74   and name HA  ))
     2.800     2.000     2.000 peak 10491 weight  0.11000E+01 volume  0.36339E+03 ppm1      7.996 ppm2      4.370
ASSI (10511)
   (( segid "BrD " and resid 54   and name HN  ))
   (( segid "BrD " and resid 53   and name HB1 ))
     2.800     2.000     2.000 peak 10511 weight  0.11000E+01 volume  0.43885E+03 ppm1      9.037 ppm2      2.816
ASSI (10521)
   (( segid "BrD " and resid 54   and name HN  ))
   (  segid "BrD " and resid 50   and name HG2%)
     3.400     2.900     2.100 peak 10521 weight  0.11000E+01 volume  0.12606E+03 ppm1      9.036 ppm2      0.987
ASSI (10671)
   (( segid "BrD " and resid 82   and name HN  ))
   (( segid "BrD " and resid 78   and name HA  ))
     3.900     3.800     1.600 peak 10671 weight  0.11000E+01 volume  0.53978E+02 ppm1      6.981 ppm2      4.005
ASSI (10691)
   (( segid "BrD " and resid 81   and name HN  ))
   (( segid "BrD " and resid 80   and name HG1 ))
     3.600     3.200     1.900 peak 10691 weight  0.11000E+01 volume  0.91821E+02 ppm1      7.640 ppm2      2.349
ASSI (10701)
   (( segid "BrD " and resid 81   and name HN  ))
   (( segid "BrD " and resid 80   and name HB1 ))
     3.700     3.400     1.800 peak 10701 weight  0.11000E+01 volume  0.72987E+02 ppm1      7.640 ppm2      2.580
ASSI (10711)
   (( segid "BrD " and resid 81   and name HN  ))
   (( segid "BrD " and resid 80   and name HB2 ))
     3.700     3.400     1.800 peak 10711 weight  0.11000E+01 volume  0.72825E+02 ppm1      7.640 ppm2      2.493
ASSI (10731)
   (( segid "BrD " and resid 81   and name HN  ))
   (( segid "BrD " and resid 79   and name HA  ))
     3.900     3.800     1.600 peak 10731 weight  0.11000E+01 volume  0.55498E+02 ppm1      7.640 ppm2      4.412
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ASSI (10791)
   (( segid "BrD " and resid 80   and name HN  ))
   (  segid "BrD " and resid 76   and name HD2%)
     5.500     5.500     0.000 peak 10791 weight  0.11000E+01 volume  0.63252E+00 ppm1      8.014 ppm2      0.660
ASSI (10801)
   (( segid "BrD " and resid 80   and name HN  ))
   (  segid "BrD " and resid 76   and name HD1%)
     4.400     4.400     1.100 peak 10801 weight  0.11000E+01 volume  0.27938E+02 ppm1      8.014 ppm2      0.791
ASSI (10831)
   (( segid "BrD " and resid 79   and name HN  ))
   (( segid "BrD " and resid 76   and name HB1 ))
     3.300     2.700     2.200 peak 10831 weight  0.11000E+01 volume  0.14525E+03 ppm1      8.680 ppm2      1.364
ASSI (10911)
   (( segid "BrD " and resid 86   and name HN  ))
   (( segid "BrD " and resid 83   and name HA  ))
     3.300     2.700     2.200 peak 10911 weight  0.11000E+01 volume  0.16077E+03 ppm1      8.423 ppm2      4.445
ASSI (10951)
   (( segid "BrD " and resid 87   and name HN  ))
   (( segid "BrD " and resid 86   and name HD1 ))
     3.500     3.100     2.000 peak 10951 weight  0.11000E+01 volume  0.10535E+03 ppm1      8.571 ppm2      1.898
ASSI (10961)
   (( segid "BrD " and resid 86   and name HN  ))
   (( segid "BrD " and resid 87   and name HN  ))
     3.100     2.400     2.400 peak 10961 weight  0.11000E+01 volume  0.19900E+03 ppm1      8.424 ppm2      8.553
ASSI (10971)
   (( segid "BrD " and resid 87   and name HN  ))
   (( segid "BrD " and resid 83   and name HA  ))
     4.200     4.200     1.300 peak 10971 weight  0.11000E+01 volume  0.36593E+02 ppm1      8.572 ppm2      4.445
ASSI (11061)
   (( segid "BrD " and resid 89   and name HN  ))
   (  segid "BrD " and resid 88   and name HD% )
     3.200     2.600     2.300 peak 11061 weight  0.11000E+01 volume  0.19134E+03 ppm1      8.858 ppm2      7.596
ASSI (11071)
   (( segid "BrD " and resid 89   and name HN  ))
   (( segid "BrD " and resid 91   and name HD1 ))
     5.300     5.300     0.200 peak 11071 weight  0.11000E+01 volume  0.89575E+01 ppm1      8.858 ppm2      4.559
ASSI (11081)
   (( segid "BrD " and resid 89   and name HN  ))
   (( segid "BrD " and resid 91   and name HD2 ))
     3.800     3.600     1.700 peak 11081 weight  0.11000E+01 volume  0.66703E+02 ppm1      8.858 ppm2      4.400
ASSI (11101)
   (( segid "BrD " and resid 89   and name HN  ))
   (( segid "BrD " and resid 87   and name HB1 ))
     3.800     3.600     1.700 peak 11101 weight  0.11000E+01 volume  0.67773E+02 ppm1      8.858 ppm2      2.779
ASSI (11111)
   (( segid "BrD " and resid 89   and name HN  ))
   (( segid "BrD " and resid 87   and name HB2 ))
     4.200     4.200     1.300 peak 11111 weight  0.11000E+01 volume  0.36189E+02 ppm1      8.865 ppm2      2.610
ASSI (11121)
   (( segid "BrD " and resid 92   and name HN  ))
   (( segid "BrD " and resid 91   and name HB1 ))
     3.200     2.600     2.300 peak 11121 weight  0.11000E+01 volume  0.16770E+03 ppm1      8.876 ppm2      3.059
ASSI (11221)
   (( segid "BrD " and resid 30   and name HN  ))
   (( segid "BrD " and resid 28   and name HN  ))
     4.100     4.100     1.400 peak 11221 weight  0.11000E+01 volume  0.38088E+02 ppm1     12.275 ppm2      8.143
ASSI (11261)
   (( segid "BrD " and resid 31   and name HN  ))
   (( segid "BrD " and resid 29   and name HG1 ))
     5.100     5.100     0.400 peak 11261 weight  0.11000E+01 volume  0.11011E+02 ppm1      8.486 ppm2      2.997
ASSI (11311)
   (( segid "BrD " and resid 31   and name HN  ))
   (  segid "BrD " and resid 102  and name HD1%)
     3.300     2.700     2.200 peak 11311 weight  0.11000E+01 volume  0.14151E+03 ppm1      8.480 ppm2      1.314
ASSI (11331)
   (( segid "BrD " and resid 32   and name HN  ))
   (( segid "BrD " and resid 33   and name HD1 ))
     3.900     3.800     1.600 peak 11331 weight  0.11000E+01 volume  0.57286E+02 ppm1      7.738 ppm2      2.762
ASSI (11341)
   (( segid "BrD " and resid 32   and name HN  ))
   (( segid "BrD " and resid 33   and name HD2 ))
     2.500     1.600     1.600 peak 11341 weight  0.11000E+01 volume  0.82617E+03 ppm1      7.739 ppm2      2.174
ASSI (11381)
   (( segid "BrD " and resid 34   and name HN  ))
   (( segid "BrD " and resid 32   and name HA  ))
     4.200     4.200     1.300 peak 11381 weight  0.11000E+01 volume  0.36612E+02 ppm1      8.183 ppm2      4.975
ASSI (11411)
   (( segid "BrD " and resid 34   and name HN  ))
   (( segid "BrD " and resid 33   and name HD1 ))
     2.600     1.700     1.700 peak 11411 weight  0.11000E+01 volume  0.60528E+03 ppm1      8.181 ppm2      2.784
ASSI (11421)
   (( segid "BrD " and resid 34   and name HN  ))
   (( segid "BrD " and resid 33   and name HD2 ))
     3.300     2.700     2.200 peak 11421 weight  0.11000E+01 volume  0.15559E+03 ppm1      8.184 ppm2      2.174
ASSI (11461)
   (( segid "BrD " and resid 34   and name HN  ))
   (( segid "BrD " and resid 33   and name HB1 ))
     3.500     3.100     2.000 peak 11461 weight  0.11000E+01 volume  0.11065E+03 ppm1      8.178 ppm2      1.094
ASSI (11471)
   (( segid "BrD " and resid 34   and name HN  ))
   (( segid "BrD " and resid 33   and name HG1 ))
     4.100     4.100     1.400 peak 11471 weight  0.11000E+01 volume  0.41672E+02 ppm1      8.177 ppm2      0.840
ASSI (11481)
   (( segid "BrD " and resid 34   and name HN  ))
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   (( segid "BrD " and resid 33   and name HA  ))
      3.200      2.600      2.300 peak 11481 weight  0.11000E+01 volume  0.17351E+03 ppm1      8.182 ppm2      4.363
ASSI (11501)
   (( segid "BrD " and resid 36   and name HN  ))
   (( segid "BrD " and resid 35   and name HB1 ))
      4.000      4.000      1.500 peak 11501 weight  0.11000E+01 volume  0.43329E+02 ppm1      8.308 ppm2      2.840
ASSI (11611)
   (( segid "BrD " and resid 67   and name HN  ))
   (( segid "BrD " and resid 65   and name HB2 ))
      3.800      3.600      1.700 peak 11611 weight  0.11000E+01 volume  0.63235E+02 ppm1      8.832 ppm2      3.380
ASSI (11621)
   (( segid "BrD " and resid 67   and name HN  ))
   (( segid "BrD " and resid 66   and name HG1 ))
      3.700      3.400      1.800 peak 11621 weight  0.11000E+01 volume  0.76792E+02 ppm1      8.832 ppm2      2.146
ASSI (11641)
   (( segid "BrD " and resid 68   and name HN  ))
   (( segid "BrD " and resid 66   and name HA  ))
      2.500      1.600      1.600 peak 11641 weight  0.11000E+01 volume  0.80687E+03 ppm1      8.626 ppm2      5.012
ASSI (11681)
   (( segid "BrD " and resid 68   and name HN  ))
   (  segid "BrD " and resid 69   and name HG2% )
      3.400      2.900      2.100 peak 11681 weight  0.11000E+01 volume  0.13257E+03 ppm1      8.626 ppm2      1.437
ASSI (11691)
   (( segid "BrD " and resid 68   and name HN  ))
   (  segid "BrD " and resid 69   and name HG1% )
      3.700      3.400      1.800 peak 11691 weight  0.11000E+01 volume  0.73874E+02 ppm1      8.626 ppm2      1.562
ASSI (11721)
   (( segid "BrD " and resid 69   and name HN  ))
   (  segid "BrD " and resid 68   and name HD% )
      3.500      3.100      2.000 peak 11721 weight  0.11000E+01 volume  0.11106E+03 ppm1      8.306 ppm2      7.782
ASSI (11781)
   (( segid "BrD " and resid 70   and name HN  ))
   (( segid "BrD " and resid 68   and name HA  ))
      3.200      2.600      2.300 peak 11781 weight  0.11000E+01 volume  0.19118E+03 ppm1      8.039 ppm2      5.135
ASSI (11791)
   (( segid "BrD " and resid 74   and name HN  ))
   (  segid "BrD " and resid 73   and name HD2% )
      4.400      4.400      1.100 peak 11791 weight  0.11000E+01 volume  0.24720E+02 ppm1      7.536 ppm2      1.502
ASSI (11801)
   (( segid "BrD " and resid 74   and name HN  ))
   (  segid "BrD " and resid 73   and name HD1% )
      4.100      4.100      1.400 peak 11801 weight  0.11000E+01 volume  0.39673E+02 ppm1      7.536 ppm2      1.531
ASSI (11811)
   (( segid "BrD " and resid 74   and name HN  ))
   (( segid "BrD " and resid 73   and name HG  ))
      3.100      2.400      2.400 peak 11811 weight  0.11000E+01 volume  0.21474E+03 ppm1      7.537 ppm2      2.401
ASSI (11821)
   (( segid "BrD " and resid 74   and name HN  ))
   (( segid "BrD " and resid 73   and name HB2 ))
      2.900      2.100      2.100 peak 11821 weight  0.11000E+01 volume  0.29959E+03 ppm1      7.536 ppm2      2.498
ASSI (11831)
   (( segid "BrD " and resid 74   and name HN  ))
   (( segid "BrD " and resid 73   and name HB1 ))
      3.000      2.200      2.200 peak 11831 weight  0.11000E+01 volume  0.27375E+03 ppm1      7.537 ppm2      2.603
ASSI (11871)
   (( segid "BrD " and resid 73   and name HN  ))
   (  segid "BrD " and resid 76   and name HB% )
      3.300      2.700      2.200 peak 11871 weight  0.11000E+01 volume  0.13672E+03 ppm1      8.046 ppm2      2.116
ASSI (11901)
   (( segid "BrD " and resid 74   and name HN  ))
   (  segid "BrD " and resid 18   and name HD1% )
      3.700      3.400      1.800 peak 11901 weight  0.11000E+01 volume  0.74433E+02 ppm1      7.536 ppm2      1.076
ASSI (11981)
   (( segid "BrD " and resid 98   and name HN  ))
   (( segid "BrD " and resid 97   and name HB1 ))
      2.500      1.600      1.600 peak 11981 weight  0.11000E+01 volume  0.78973E+03 ppm1      9.125 ppm2      2.698
ASSI (11991)
   (( segid "BrD " and resid 98   and name HN  ))
   (( segid "BrD " and resid 97   and name HG1 ))
      3.100      2.400      2.400 peak 11991 weight  0.11000E+01 volume  0.20137E+03 ppm1      9.125 ppm2      2.426
ASSI (12001)
   (( segid "BrD " and resid 98   and name HN  ))
   (( segid "BrD " and resid 97   and name HG2 ))
      3.100      2.400      2.400 peak 12001 weight  0.11000E+01 volume  0.20070E+03 ppm1      9.124 ppm2      2.189
ASSI (12171)
   (( segid "BrD " and resid 101  and name HN  ))
   (( segid "BrD " and resid 99   and name HA  ))
      4.000      4.000      1.500 peak 12171 weight  0.11000E+01 volume  0.46069E+02 ppm1      8.513 ppm2      4.447
ASSI (12181)
   (( segid "BrD " and resid 101  and name HN  ))
   (( segid "BrD " and resid 97   and name HA  ))
      3.100      2.400      2.400 peak 12181 weight  0.11000E+01 volume  0.20943E+03 ppm1      8.513 ppm2      4.811
ASSI (12191)
   (( segid "BrD " and resid 103  and name HN  ))
   (( segid "BrD " and resid 102  and name HB1 ))
      2.800      2.000      2.000 peak 12191 weight  0.11000E+01 volume  0.37773E+03 ppm1      8.696 ppm2      2.012
ASSI (12201)
   (( segid "BrD " and resid 104  and name HN  ))
   (( segid "BrD " and resid 100  and name HA  ))
      3.200      2.600      2.300 peak 12201 weight  0.11000E+01 volume  0.18477E+03 ppm1      7.763 ppm2      4.936
ASSI (12231)
   (( segid "BrD " and resid 107  and name HN  ))
   (( segid "BrD " and resid 104  and name HA  ))
      3.000      2.200      2.200 peak 12231 weight  0.11000E+01 volume  0.26295E+03 ppm1      8.981 ppm2      4.682
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ASSI (12321)
   (( segid "BrD " and resid 110  and name HN  ))
   (( segid "BrD " and resid 109  and name HD1 ))
      3.500      3.100      2.000 peak 12321 weight  0.11000E+01 volume  0.10959E+03 ppm1      8.714 ppm2      2.010
ASSI (12331)
   (( segid "BrD " and resid 110  and name HN  ))
   (( segid "BrD " and resid 109  and name HB1 ))
      2.700      1.800      1.800 peak 12331 weight  0.11000E+01 volume  0.48783E+03 ppm1      8.714 ppm2      2.337
ASSI (12341)
   (( segid "BrD " and resid 110  and name HN  ))
   (( segid "BrD " and resid 109  and name HG1 ))
      3.000      2.200      2.200 peak 12341 weight  0.11000E+01 volume  0.26294E+03 ppm1      8.714 ppm2      1.440
ASSI (12351)
   (( segid "BrD " and resid 111  and name HN  ))
   (( segid "BrD " and resid 110  and name HG12))
      3.000      2.200      2.200 peak 12351 weight  0.11000E+01 volume  0.27526E+03 ppm1      8.168 ppm2      1.680
ASSI (12361)
   (( segid "BrD " and resid 112  and name HN  ))
   (( segid "BrD " and resid 111  and name HG2 ))
      3.200      2.600      2.300 peak 12361 weight  0.11000E+01 volume  0.16739E+03 ppm1      8.668 ppm2      1.909
ASSI (12371)
   (( segid "BrD " and resid 113  and name HN  ))
   (( segid "BrD " and resid 110  and name HA  ))
      3.600      3.200      1.900 peak 12371 weight  0.11000E+01 volume  0.80563E+02 ppm1      8.217 ppm2      4.425
ASSI (12381)
   (( segid "BrD " and resid 113  and name HN  ))
   (( segid "BrD " and resid 111  and name HB1 ))
      3.900      3.800      1.600 peak 12381 weight  0.11000E+01 volume  0.57596E+02 ppm1      8.219 ppm2      2.486
ASSI (12391)
   (( segid "BrD " and resid 113  and name HN  ))
   (( segid "BrD " and resid 111  and name HB2 ))
      3.800      3.600      1.700 peak 12391 weight  0.11000E+01 volume  0.67480E+02 ppm1      8.218 ppm2      2.364
ASSI (12531)
   (( segid "BrD " and resid 48   and name HN  ))
   (( segid "BrD " and resid 47   and name HB1 ))
      4.300      4.300      1.200 peak 12531 weight  0.11000E+01 volume  0.28319E+02 ppm1      8.307 ppm2      1.796
ASSI (12541)
   (( segid "BrD " and resid 48   and name HN  ))
   (( segid "BrD " and resid 46   and name HA  ))
      4.000      4.000      1.500 peak 12541 weight  0.11000E+01 volume  0.44246E+02 ppm1      8.307 ppm2      4.182
ASSI (12551)
   (( segid "BrD " and resid 48   and name HN  ))
   (( segid "BrD " and resid 47   and name HB2 ))
      4.200      4.200      1.300 peak 12551 weight  0.11000E+01 volume  0.35395E+02 ppm1      8.307 ppm2      3.408
ASSI (12561)
   (( segid "BrD " and resid 47   and name HN  ))
   (  segid "BrD " and resid 46   and name HD% )
      3.500      3.100      2.000 peak 12561 weight  0.11000E+01 volume  0.10097E+03 ppm1      8.832 ppm2      5.727
ASSI (12571)
   (( segid "BrD " and resid 47   and name HN  ))
   (  segid "BrD " and resid 47   and name HD% )
      3.100      2.400      2.400 peak 12571 weight  0.11000E+01 volume  0.23274E+03 ppm1      8.833 ppm2      7.944
ASSI (12631)
   (( segid "BrD " and resid 51   and name HN  ))
   (( segid "BrD " and resid 50   and name HA  ))
      2.600      1.700      1.700 peak 12631 weight  0.11000E+01 volume  0.65616E+03 ppm1      8.377 ppm2      4.523
ASSI (12641)
   (( segid "BrD " and resid 52   and name HN  ))
   (( segid "BrD " and resid 51   and name HB1 ))
      3.400      2.900      2.100 peak 12641 weight  0.11000E+01 volume  0.11270E+03 ppm1      9.003 ppm2      1.995
ASSI (12651)
   (( segid "BrD " and resid 52   and name HN  ))
   (( segid "BrD " and resid 51   and name HG1 ))
      5.500      5.500      0.000 peak 12651 weight  0.11000E+01 volume  0.88686E+00 ppm1      9.003 ppm2      1.926
ASSI (12661)
   (( segid "BrD " and resid 52   and name HN  ))
   (( segid "BrD " and resid 51   and name HG2 ))
      3.400      2.900      2.100 peak 12661 weight  0.11000E+01 volume  0.11315E+03 ppm1      9.003 ppm2      1.780
ASSI (12671)
   (( segid "BrD " and resid 52   and name HN  ))
   (( segid "BrD " and resid 51   and name HB2 ))
      3.200      2.600      2.300 peak 12671 weight  0.11000E+01 volume  0.16847E+03 ppm1      9.004 ppm2      1.818
ASSI (12681)
   (( segid "BrD " and resid 52   and name HN  ))
   (  segid "BrD " and resid 50   and name HG2% )
      2.800      2.000      2.000 peak 12681 weight  0.11000E+01 volume  0.38955E+03 ppm1      9.002 ppm2      0.991
ASSI (12731)
   (( segid "BrD " and resid 42   and name HN  ))
   (( segid "BrD " and resid 41   and name HA  ))
      3.400      2.900      2.100 peak 12731 weight  0.11000E+01 volume  0.12554E+03 ppm1      7.822 ppm2      4.650
ASSI (12771)
   (( segid "BrD " and resid 42   and name HN  ))
   (  segid "BrD " and resid 41   and name HG2% )
      4.200      4.200      1.300 peak 12771 weight  0.11000E+01 volume  0.34295E+02 ppm1      7.821 ppm2      1.874
ASSI (12781)
   (( segid "BrD " and resid 97   and name HN  ))
   (  segid "BrD " and resid 96   and name HD% )
      3.300      2.700      2.200 peak 12781 weight  0.11000E+01 volume  0.13710E+03 ppm1      8.674 ppm2      7.701
ASSI (12791)
   (( segid "BrD " and resid 20   and name HN  ))
   (( segid "BrD " and resid 19   and name HG1 ))
      3.400      2.900      2.100 peak 12791 weight  0.11000E+01 volume  0.11346E+03 ppm1      8.146 ppm2      1.887
ASSI (12801)
   (( segid "BrD " and resid 19   and name HN  ))
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   (( segid "BrD " and resid 18   and name HB2 ))
    3.400     2.900     2.100 peak 12801 weight  0.11000E+01 volume  0.11595E+03 ppm1      9.186 ppm2      0.901
ASSI {12811}
   (( segid "BrD " and resid 19   and name HN  ))
   ( segid "BrD " and resid 63   and name HD1%)
    3.100     2.400     2.400 peak 12811 weight  0.11000E+01 volume  0.22952E+03 ppm1      9.186 ppm2      1.642
ASSI {12821}
   (( segid "BrD " and resid 19   and name HN  ))
   ( segid "BrD " and resid 63   and name HD2%)
    3.000     2.200     2.200 peak 12821 weight  0.11000E+01 volume  0.27823E+03 ppm1      9.187 ppm2      1.476
ASSI {12831}
   (( segid "BrD " and resid 19   and name HN  ))
   (( segid "BrD " and resid 16   and name HA  ))
    3.000     2.200     2.200 peak 12831 weight  0.11000E+01 volume  0.27123E+03 ppm1      9.187 ppm2      4.516
ASSI {12871}
   (( segid "BrD " and resid 20   and name HN  ))
   (( segid "BrD " and resid 18   and name HG  ))
    3.800     3.600     1.700 peak 12871 weight  0.11000E+01 volume  0.64336E+02 ppm1      8.147 ppm2      2.290
ASSI {12931}
   (( segid "BrD " and resid 23   and name HN  ))
   (( segid "BrD " and resid 22   and name HB1 ))
    2.600     1.700     1.700 peak 12931 weight  0.11000E+01 volume  0.65708E+03 ppm1      9.120 ppm2      2.697
ASSI {12941}
   (( segid "BrD " and resid 23   and name HN  ))
   (( segid "BrD " and resid 22   and name HB2 ))
    2.800     2.000     2.000 peak 12941 weight  0.11000E+01 volume  0.39331E+03 ppm1      9.122 ppm2      2.310
ASSI {13051}
   (( segid "BrD " and resid 27   and name HN  ))
   (( segid "BrD " and resid 26   and name HD1 ))
    2.700     1.800     1.800 peak 13051 weight  0.11000E+01 volume  0.67384E+03 ppm1      8.168 ppm2      2.127
ASSI {13071}
   (( segid "BrD " and resid 27   and name HN  ))
   (( segid "BrD " and resid 24   and name HG1 ))
    3.500     3.100     2.000 peak 13071 weight  0.11000E+01 volume  0.10804E+03 ppm1      8.170 ppm2      3.447
ASSI {13081}
   (( segid "BrD " and resid 27   and name HN  ))
   (( segid "BrD " and resid 24   and name HG2 ))
    3.700     3.400     1.800 peak 13081 weight  0.11000E+01 volume  0.74378E+02 ppm1      8.170 ppm2      3.074
ASSI {13141}
   (( segid "BrD " and resid 60   and name HN  ))
   (( segid "BrD " and resid 59   and name HB2 ))
    2.900     2.100     2.100 peak 13141 weight  0.11000E+01 volume  0.32659E+03 ppm1      8.565 ppm2      2.522
ASSI {13151}
   (( segid "BrD " and resid 65   and name HN  ))
   (( segid "BrD " and resid 64   and name HG1 ))
    3.300     2.700     2.200 peak 13151 weight  0.11000E+01 volume  0.14156E+03 ppm1      8.565 ppm2      2.203
ASSI {13211}
   (( segid "BrD " and resid 15   and name HN  ))
   (( segid "BrD " and resid 14   and name HG  ))
    3.700     3.400     1.800 peak 13211 weight  0.11000E+01 volume  0.73008E+02 ppm1      8.597 ppm2      2.087
ASSI {13281}
   (( segid "BrD " and resid 65   and name HD21))
   (( segid "BrD " and resid 64   and name HB1 ))
    3.600     3.200     1.900 peak 13281 weight  0.11000E+01 volume  0.89819E+02 ppm1      8.205 ppm2      2.662
ASSI {13291}
   (( segid "BrD " and resid 65   and name HD22))
   (( segid "BrD " and resid 64   and name HB1 ))
    3.600     3.200     1.900 peak 13291 weight  0.11000E+01 volume  0.84418E+02 ppm1      7.576 ppm2      2.662
ASSI {13321}
   (( segid "BrD " and resid 93   and name HN  ))
   (( segid "BrD " and resid 93   and name HB1 ))
    4.100     4.100     1.400 peak 13321 weight  0.11000E+01 volume  0.42284E+02 ppm1      8.713 ppm2      5.009
ASSI {13331}
   (( segid "BrD " and resid 94   and name HN  ))
   (( segid "BrD " and resid 93   and name HB1 ))
    3.700     3.400     1.800 peak 13331 weight  0.11000E+01 volume  0.78957E+02 ppm1      9.679 ppm2      5.000
ASSI {13341}
   (( segid "BrD " and resid 17   and name HN  ))
   (( segid "BrD " and resid 16   and name HB1 ))
    3.400     2.900     2.100 peak 13341 weight  0.11000E+01 volume  0.11732E+03 ppm1      8.670 ppm2      4.602
ASSI {13351}
   (( segid "BrD " and resid 62   and name HN  ))
   (( segid "BrD " and resid 62   and name HD2 ))
    2.700     1.800     1.800 peak 13351 weight  0.11000E+01 volume  0.44005E+03 ppm1      8.998 ppm2      2.658
ASSI {13361}
   (( segid "BrD " and resid 86   and name HN  ))
   (( segid "BrD " and resid 86   and name HG1 ))
    4.100     4.100     1.400 peak 13361 weight  0.11000E+01 volume  0.42972E+02 ppm1      8.423 ppm2      1.920
ASSI {13371}
   (( segid "BrD " and resid 17   and name HN  ))
   (( segid "BrD " and resid 14   and name HA  ))
    3.600     1.700     1.700 peak 13371 weight  0.11000E+01 volume  0.66944E+03 ppm1      8.670 ppm2      4.652
ASSI {13381}
   (( segid "BrD " and resid 18   and name HN  ))
   (( segid "BrD " and resid 15   and name HA  ))
    3.800     3.600     1.700 peak 13381 weight  0.11000E+01 volume  0.66429E+02 ppm1      9.073 ppm2      4.620
ASSI {13391}
   (( segid "BrD " and resid 19   and name HN  ))
   (( segid "BrD " and resid 18   and name HN  ))
    2.300     1.300     1.300 peak 13391 weight  0.11000E+01 volume  0.12618E+04 ppm1      9.186 ppm2      9.067
ASSI {13401}
   (( segid "BrD " and resid 59   and name HN  ))
   (( segid "BrD " and resid 56   and name HA  ))
    3.100     2.400     2.400 peak 13401 weight  0.11000E+01 volume  0.22047E+03 ppm1      8.498 ppm2      4.643
ASSI {13421}
   (( segid "BrD " and resid 79   and name HN  ))
   (( segid "BrD " and resid 75   and name HA  ))
    4.000     4.000     1.500 peak 13421 weight  0.11000E+01 volume  0.47743E+02 ppm1      8.680 ppm2      4.518
ASSI {13431}
   (( segid "BrD " and resid 81   and name HN  ))
   (( segid "BrD " and resid 77   and name HA  ))
    4.500     4.500     1.000 peak 13431 weight  0.11000E+01 volume  0.23511E+02 ppm1      7.639 ppm2      4.978
ASSI {13441}
   (( segid "BrD " and resid 85   and name HN  ))
   (( segid "BrD " and resid 83   and name HA  ))
    3.600     3.200     1.900 peak 13441 weight  0.11000E+01 volume  0.85635E+02 ppm1      7.519 ppm2      4.441
ASSI {13451}
   (( segid "BrD " and resid 85   and name HN  ))
   (( segid "BrD " and resid 81   and name HA  ))
    2.500     1.600     1.600 peak 13451 weight  0.11000E+01 volume  0.75325E+03 ppm1      7.517 ppm2      3.646
ASSI {13461}
   (( segid "BrD " and resid 88   and name HN  ))
   (( segid "BrD " and resid 84   and name HA  ))
    2.800     2.000     2.000 peak 13461 weight  0.11000E+01 volume  0.40309E+03 ppm1      8.357 ppm2      4.922
ASSI {13481}
   (( segid "BrD " and resid 81   and name HN  ))
   (( segid "BrD " and resid 83   and name HN  ))
    3.900     3.800     1.600 peak 13481 weight  0.11000E+01 volume  0.80469E+02 ppm1      7.640 ppm2      9.655
ASSI {13491}
   (( segid "BrD " and resid 96   and name HN  ))
   (( segid "BrD " and resid 93   and name HA  ))
    3.700     3.400     1.800 peak 13491 weight  0.11000E+01 volume  0.70852E+02 ppm1      7.981 ppm2      5.013
ASSI {13501}
   (( segid "BrD " and resid 109  and name HN  ))
   (( segid "BrD " and resid 105  and name HA  ))
    4.600     4.600     0.900 peak 13501 weight  0.11000E+01 volume  0.18885E+02 ppm1      8.574 ppm2      4.935
ASSI {13511}
   (( segid "BrD " and resid 110  and name HN  ))
   (( segid "BrD " and resid 108  and name HA  ))
    3.500     3.100     2.000 peak 13511 weight  0.11000E+01 volume  0.11166E+03 ppm1      8.714 ppm2      4.818
ASSI {13521}
   (( segid "BrD " and resid 92   and name HN  ))
   (( segid "BrD " and resid 91   and name HA  ))
    3.200     2.600     2.300 peak 13521 weight  0.11000E+01 volume  0.16456E+03 ppm1      8.873 ppm2      5.343
ASSI {13541}
   (( segid "BrD " and resid 98   and name HN  ))
   (( segid "BrD " and resid 100  and name HN  ))
    2.900     2.100     2.100 peak 13541 weight  0.11000E+01 volume  0.30894E+03 ppm1      9.125 ppm2      8.653
ASSI {13551}
   (( segid "BrD " and resid 103  and name HN  ))
   (( segid "BrD " and resid 101  and name HN  ))
    2.900     2.100     2.100 peak 13551 weight  0.11000E+01 volume  0.34725E+03 ppm1      8.696 ppm2      8.519
ASSI {13561}
   (( segid "BrD " and resid 32   and name HN  ))
   (( segid "BrD " and resid 30   and name HA  ))
    4.400     4.400     1.100 peak 13561 weight  0.11000E+01 volume  0.25941E+02 ppm1      7.739 ppm2      5.445
ASSI {13571}
   (( segid "BrD " and resid 24   and name HN  ))
   (( segid "BrD " and resid 23   and name HB2 ))
    2.800     2.000     2.000 peak 13571 weight  0.11000E+01 volume  0.42825E+03 ppm1      8.659 ppm2      2.870
ASSI {13581}
   (( segid "BrD " and resid 73   and name HN  ))
   (( segid "BrD " and resid 75   and name HN  ))
    4.000     4.000     1.500 peak 13581 weight  0.11000E+01 volume  0.46662E+02 ppm1      8.045 ppm2      9.084
ASSI {13591}
   (( segid "BrD " and resid 62   and name HN  ))
   (( segid "BrD " and resid 61   and name HG1 ))
    3.900     3.800     1.600 peak 13591 weight  0.11000E+01 volume  0.54843E+02 ppm1      8.999 ppm2      2.952
ASSI {13611}
   (( segid "BrD " and resid 67   and name HN  ))
   (( segid "BrD " and resid 65   and name HB1 ))
    2.800     2.000     2.000 peak 13611 weight  0.11000E+01 volume  0.36617E+03 ppm1      8.832 ppm2      3.626
ASSI {13621}
   (( segid "BrD " and resid 75   and name HN  ))
   (( segid "BrD " and resid 74   and name HB2 ))
    3.200     2.600     2.300 peak 13621 weight  0.11000E+01 volume  0.17250E+03 ppm1      9.106 ppm2      2.988
ASSI {13641}
   (( segid "BrD " and resid 104  and name HN  ))
   (( segid "BrD " and resid 106  and name HN  ))
    4.900     4.900     0.600 peak 13641 weight  0.11000E+01 volume  0.14134E+02 ppm1      7.763 ppm2      9.736
ASSI {13671}
   (( segid "BrD " and resid 74   and name HN  ))
   ( segid "BrD " and resid 18   and name HD2%)
    3.900     3.800     1.600 peak 13671 weight  0.11000E+01 volume  0.56031E+02 ppm1      7.545 ppm2      0.414
ASSI {13701}
   (( segid "BrD " and resid 61   and name HN  ))
   (( segid "BrD " and resid 61   and name HB1 ))
    2.800     2.000     2.000 peak 13701 weight  0.11000E+01 volume  0.41690E+03 ppm1      8.743 ppm2      2.837
ASSI {13711}
   (( segid "BrD " and resid 62   and name HN  ))
   (( segid "BrD " and resid 61   and name HB1 ))
    2.800     2.000     2.000 peak 13711 weight  0.11000E+01 volume  0.40898E+03 ppm1      8.998 ppm2      2.653
ASSI {13731}
   (( segid "BrD " and resid 25   and name HN  ))
   (( segid "BrD " and resid 21   and name HA  ))
    2.900     2.100     2.100 peak 13731 weight  0.11000E+01 volume  0.30325E+03 ppm1      9.134 ppm2      4.393
ASSI {13741}
   (( segid "BrD " and resid 63   and name HN  ))
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   (( segid "BrD " and resid 59   and name HA  ))
     3.200      2.600      2.300 peak 13741 weight  0.11000E+01 volume  0.16317E+03 ppm1      9.472 ppm2      4.926
ASSI {13761}
   (( segid "BrD " and resid 74   and name HN  ))
   (( segid "BrD " and resid 71   and name HA  ))
     3.200      2.600      2.300 peak 13761 weight  0.11000E+01 volume  0.19208E+03 ppm1      7.536 ppm2      4.622
ASSI {13771}
   (( segid "BrD " and resid 75   and name HN  ))
   (( segid "BrD " and resid 71   and name HA  ))
     3.100      2.600      2.400 peak 13771 weight  0.11000E+01 volume  0.21726E+03 ppm1      9.106 ppm2      4.628
ASSI {13781}
   (( segid "BrD " and resid 77   and name HN  ))
   (( segid "BrD " and resid 74   and name HA  ))
     3.200      2.600      2.300 peak 13781 weight  0.11000E+01 volume  0.16504E+03 ppm1      7.996 ppm2      4.371
ASSI {13791}
   (( segid "BrD " and resid 105  and name HN  ))
   (( segid "BrD " and resid 101  and name HA  ))
     3.200      2.600      2.300 peak 13791 weight  0.11000E+01 volume  0.19414E+03 ppm1      8.487 ppm2      4.253
ASSI {13801}
   (( segid "BrD " and resid 26   and name HN  ))
   (( segid "BrD " and resid 24   and name HA  ))
     3.900      3.800      1.600 peak 13801 weight  0.11000E+01 volume  0.52793E+02 ppm1      9.196 ppm2      4.755
ASSI {13811}
   (( segid "BrD " and resid 26   and name HN  ))
   (( segid "BrD " and resid 25   and name HA  ))
     3.800      3.600      1.700 peak 13811 weight  0.11000E+01 volume  0.62704E+02 ppm1      9.196 ppm2      4.415
ASSI {13821}
   (( segid "BrD " and resid 29   and name HN  ))
   (( segid "BrD " and resid 25   and name HA  ))
     5.500      5.500      0.000 peak 13821 weight  0.11000E+01 volume  0.27795E-01 ppm1      9.152 ppm2      4.451
ASSI {13831}
   (( segid "BrD " and resid 54   and name HN  ))
   (( segid "BrD " and resid 55   and name HN  ))
     2.900      2.100      2.100 peak 13831 weight  0.11000E+01 volume  0.31830E+03 ppm1      9.037 ppm2      7.972
ASSI {13851}
   (( segid "BrD " and resid 48   and name HN  ))
   (  segid "BrD " and resid 47   and name HD% )
     3.900      3.800      1.600 peak 13851 weight  0.11000E+01 volume  0.57580E+02 ppm1      8.307 ppm2      7.949
ASSI {13861}
   (( segid "BrD " and resid 96   and name HN  ))
   (  segid "BrD " and resid 95   and name HD% )
     3.500      3.100      2.000 peak 13861 weight  0.11000E+01 volume  0.10869E+03 ppm1      7.979 ppm2      7.498
ASSI {14011}
   (( segid "BrD " and resid 108  and name HN  ))
   (  segid "BrD " and resid 107  and name HD% )
     4.300      4.300      1.200 peak 14011 weight  0.11000E+01 volume  0.30492E+02 ppm1      8.528 ppm2      7.782
ASSI {14881}
   (( segid "BrD " and resid 54   and name HN  ))
   (( segid "BrD " and resid 54   and name HG1 ))
     4.500      4.500      1.000 peak 14881 weight  0.11000E+01 volume  0.23500E+02 ppm1      9.038 ppm2      3.297
ASSI {15591}
   (( segid "BrD " and resid 32   and name HE1 ))
   (( segid "BrD " and resid 32   and name HB2 ))
     4.000      4.000      1.500 peak 15591 weight  0.11000E+01 volume  0.47456E+02 ppm1     11.081 ppm2      3.958
ASSI {15601}
   (( segid "BrD " and resid 32   and name HE1 ))
   (( segid "BrD " and resid 32   and name HB1 ))
     5.200      5.200      0.300 peak 15601 weight  0.11000E+01 volume  0.94290E+01 ppm1     11.081 ppm2      4.201
ASSI {  111}
   (( segid "BrD " and resid 99   and name HN  ))
   (( segid "BrD " and resid 34   and name HZ  ))
     3.100      2.400      2.400 peak  111 weight  0.10000E+01 volume  0.20460E+03 ppm1      8.936 ppm2      7.899
ASSI {  801}
   (( segid "BrD " and resid 97   and name HN  ))
   (( segid "BrD " and resid 97   and name HE1 ))
     4.000      4.000      1.500 peak  801 weight  0.10000E+01 volume  0.47904E+02 ppm1      8.673 ppm2      3.572
ASSI {  931}
   (( segid "BrD " and resid 117  and name HN  ))
   (( segid "BrD " and resid 116  and name HN  ))
     3.500      3.100      2.000 peak  931 weight  0.10000E+01 volume  0.10704E+03 ppm1      8.883 ppm2      8.075
ASSI { 1891}
   (( segid "BrD " and resid 83   and name HN  ))
   (( segid "BrD " and resid 85   and name HN  ))
     4.000      4.000      1.500 peak 1891 weight  0.10000E+01 volume  0.44105E+02 ppm1      9.660 ppm2      7.505
ASSI { 2331}
   (( segid "BrD " and resid 49   and name HN  ))
   (( segid "BrD " and resid 50   and name HA  ))
     4.000      4.000      1.500 peak 2331 weight  0.10000E+01 volume  0.49544E+02 ppm1      7.761 ppm2      4.525
ASSI { 2631}
   (( segid "BrD " and resid 103  and name HN  ))
   (  segid "BrD " and resid 82   and name HD% )
     3.800      3.600      1.700 peak 2631 weight  0.10000E+01 volume  0.64814E+02 ppm1      8.695 ppm2      7.246
ASSI { 3601}
   (( segid "BrD " and resid 9    and name HN  ))
   (( segid "BrD " and resid 9    and name HA  ))
     2.900      2.100      2.100 peak 3601 weight  0.10000E+01 volume  0.32855E+03 ppm1      9.052 ppm2      4.936
ASSI { 3751}
   (( segid "BrD " and resid 56   and name HN  ))
   (( segid "BrD " and resid 35   and name HA  ))
     3.200      2.600      2.300 peak 3751 weight  0.10000E+01 volume  0.18743E+03 ppm1      9.678 ppm2      4.895
ASSI { 4371}
   (( segid "BrD " and resid 40   and name HN  ))
   (( segid "BrD " and resid 42   and name HA  ))
     3.400      2.900      2.100 peak 4371 weight  0.10000E+01 volume  0.12104E+03 ppm1      8.662 ppm2      5.021
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ASSI { 4671}
   (( segid "BrD " and resid 61   and name HN  ))
   (( segid "BrD " and resid 60   and name HB1 ))
     2.900      2.100      2.100 peak 4671 weight  0.10000E+01 volume  0.31176E+03 ppm1      8.746 ppm2      4.992
ASSI { 5081}
   (( segid "BrD " and resid 73   and name HN  ))
   (( segid "BrD " and resid 74   and name HB2 ))
     3.100      2.400      2.400 peak 5081 weight  0.10000E+01 volume  0.21337E+03 ppm1      8.007 ppm2      3.018
ASSI { 7641}
   (( segid "BrD " and resid 76   and name HN  ))
   (( segid "BrD " and resid 73   and name HA  ))
     3.500      3.100      2.000 peak 7641 weight  0.10000E+01 volume  0.87995E+02 ppm1      8.611 ppm2      4.812
ASSI { 7691}
   (( segid "BrD " and resid 83   and name HN  ))
   (( segid "BrD " and resid 80   and name HA  ))
     2.800      2.000      2.000 peak 7691 weight  0.10000E+01 volume  0.35765E+03 ppm1      9.660 ppm2      4.675
ASSI { 8061}
   (( segid "BrD " and resid 39   and name HN  ))
   (( segid "BrD " and resid 38   and name HN  ))
     4.300      4.300      1.200 peak 8061 weight  0.10000E+01 volume  0.29321E+02 ppm1      9.651 ppm2      8.726
ASSI { 8071}
   (( segid "BrD " and resid 39   and name HN  ))
   (( segid "BrD " and resid 42   and name HG1 ))
     4.100      4.100      1.400 peak 8071 weight  0.10000E+01 volume  0.37403E+02 ppm1      9.657 ppm2      2.891
ASSI { 8081}
   (( segid "BrD " and resid 39   and name HN  ))
   (( segid "BrD " and resid 42   and name HB1 ))
     3.900      3.800      1.600 peak 8081 weight  0.10000E+01 volume  0.55108E+02 ppm1      9.658 ppm2      2.784
ASSI { 8091}
   (( segid "BrD " and resid 39   and name HN  ))
   (( segid "BrD " and resid 42   and name HB2 ))
     4.200      4.200      1.300 peak 8091 weight  0.10000E+01 volume  0.33585E+02 ppm1      9.651 ppm2      2.607
ASSI { 8141}
   (( segid "BrD " and resid 57   and name HN  ))
   (( segid "BrD " and resid 36   and name HA  ))
     3.100      2.400      2.400 peak 8141 weight  0.10000E+01 volume  0.21622E+03 ppm1      9.359 ppm2      5.440
ASSI { 8151}
   (( segid "BrD " and resid 57   and name HN  ))
   (( segid "BrD " and resid 58   and name HA  ))
     4.100      4.100      1.400 peak 8151 weight  0.10000E+01 volume  0.38316E+02 ppm1      9.359 ppm2      4.453
ASSI { 8161}
   (( segid "BrD " and resid 57   and name HN  ))
   (( segid "BrD " and resid 37   and name HD1 ))
     3.700      3.400      1.800 peak 8161 weight  0.10000E+01 volume  0.78885E+02 ppm1      9.359 ppm2      4.288
ASSI { 8221}
   (( segid "BrD " and resid 114  and name HN  ))
   (( segid "BrD " and resid 115  and name HG  ))
     3.800      3.600      1.700 peak 8221 weight  0.10000E+01 volume  0.68239E+02 ppm1      8.377 ppm2      2.169
OR { 8221}
   (( segid "BrD " and resid 114  and name HN  ))
   (( segid "BrD " and resid 115  and name HB1 ))
ASSI { 8231}
   (( segid "BrD " and resid 114  and name HN  ))
   (  segid "BrD " and resid 115  and name HD1% )
     3.700      3.400      1.800 peak 8231 weight  0.10000E+01 volume  0.72638E+02 ppm1      8.375 ppm2      1.308
ASSI { 8271}
   (( segid "BrD " and resid 28   and name HN  ))
   (  segid "BrD " and resid 31   and name HB% )
     3.400      2.900      2.100 peak 8271 weight  0.10000E+01 volume  0.12341E+03 ppm1      8.166 ppm2      2.308
ASSI { 8281}
   (( segid "BrD " and resid 28   and name HN  ))
   (( segid "BrD " and resid 26   and name HB1 ))
     3.700      3.400      1.800 peak 8281 weight  0.10000E+01 volume  0.69844E+02 ppm1      8.166 ppm2      2.476
ASSI { 8301}
   (( segid "BrD " and resid 28   and name HN  ))
   (  segid "BrD " and resid 102  and name HD1% )
     3.400      2.900      2.100 peak 8301 weight  0.10000E+01 volume  0.11542E+03 ppm1      8.166 ppm2      1.318
ASSI { 8311}
   (( segid "BrD " and resid 118  and name HN  ))
   (( segid "BrD " and resid 116  and name HG12 ))
     3.200      2.600      2.300 peak 8311 weight  0.10000E+01 volume  0.19156E+03 ppm1      8.381 ppm2      1.558
ASSI { 8321}
   (( segid "BrD " and resid 118  and name HN  ))
   (  segid "BrD " and resid 116  and name HD1% )
     4.100      4.100      1.400 peak 8321 weight  0.10000E+01 volume  0.39844E+02 ppm1      8.380 ppm2      1.394
OR { 8321}
   (( segid "BrD " and resid 118  and name HN  ))
   (  segid "BrD " and resid 116  and name HG2% )
ASSI { 8331}
   (( segid "BrD " and resid 118  and name HN  ))
   (  segid "BrD " and resid 110  and name HG2% )
     3.400      2.900      2.100 peak 8331 weight  0.10000E+01 volume  0.11494E+03 ppm1      8.381 ppm2      1.296
ASSI { 8341}
   (( segid "BrD " and resid 51   and name HN  ))
   (  segid "BrD " and resid 50   and name HD1% )
     4.000      4.000      1.500 peak 8341 weight  0.10000E+01 volume  0.45762E+02 ppm1      8.381 ppm2      1.156
ASSI { 8401}
   (( segid "BrD " and resid 38   and name HN  ))
   (( segid "BrD " and resid 37   and name HB2 ))
     3.000      2.200      2.200 peak 8401 weight  0.10000E+01 volume  0.24692E+03 ppm1      8.733 ppm2      2.290
ASSI { 8411}
   (( segid "BrD " and resid 117  and name HN  ))
   (( segid "BrD " and resid 118  and name HN  ))
     3.900      3.800      1.600 peak 8411 weight  0.10000E+01 volume  0.55844E+02 ppm1      8.880 ppm2      8.368
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ASSI { 8421}
  (( segid "BrD " and resid 117  and name HN  ))
  (( segid "BrD " and resid 116  and name HG11))
     3.900      3.800      1.600 peak  8421 weight  0.10000E+01 volume  0.57435E+02 ppm1      8.876 ppm2      1.915
ASSI { 8441}
  (( segid "BrD " and resid 7    and name HN  ))
  (( segid "BrD " and resid 6    and name HD1 ))
     3.800      3.600      1.700 peak  8441 weight  0.10000E+01 volume  0.67409E+02 ppm1      8.923 ppm2      2.338
ASSI { 8451}
  (( segid "BrD " and resid 102  and name HN  ))
  (( segid "BrD " and resid 28   and name HE1 ))
     3.900      3.800      1.600 peak  8451 weight  0.10000E+01 volume  0.51665E+02 ppm1      9.156 ppm2      8.153
ASSI { 8461}
  (( segid "BrD " and resid 102  and name HN  ))
  (  segid "BrD " and resid 82   and name HE% )
     4.100      4.100      1.400 peak  8461 weight  0.10000E+01 volume  0.42485E+02 ppm1      9.156 ppm2      7.050
OR { 8461}
  (( segid "BrD " and resid 102  and name HN  ))
  (( segid "BrD " and resid 82   and name HZ  ))
ASSI { 8481}
  (( segid "BrD " and resid 102  and name HN  ))
  (( segid "BrD " and resid 103  and name HB1 ))
     3.600      3.200      1.900 peak  8481 weight  0.10000E+01 volume  0.66913E+02 ppm1      9.156 ppm2      2.348
ASSI { 8501}
  (( segid "BrD " and resid 50   and name HN  ))
  (( segid "BrD " and resid 48   and name HA  ))
     5.100      5.100      0.400 peak  8501 weight  0.10000E+01 volume  0.11267E+02 ppm1      8.564 ppm2      4.822
ASSI { 8551}
  (( segid "BrD " and resid 46   and name HN  ))
  (( segid "BrD " and resid 44   and name HA  ))
     4.000      4.000      1.500 peak  8551 weight  0.10000E+01 volume  0.43724E+02 ppm1      8.562 ppm2      5.119
ASSI { 8581}
  (( segid "BrD " and resid 46   and name HN  ))
  (  segid "BrD " and resid 43   and name HB% )
     2.800      2.000      2.000 peak  8581 weight  0.10000E+01 volume  0.40920E+02 ppm1      8.562 ppm2      1.692
ASSI { 8601}
  (( segid "BrD " and resid 43   and name HN  ))
  (( segid "BrD " and resid 39   and name HB1 ))
     4.100      4.100      1.400 peak  8601 weight  0.10000E+01 volume  0.39702E+02 ppm1      8.001 ppm2      2.497
ASSI { 8611}
  (( segid "BrD " and resid 43   and name HN  ))
  (( segid "BrD " and resid 39   and name HD1 ))
     3.500      3.100      2.000 peak  8611 weight  0.10000E+01 volume  0.96093E+02 ppm1      8.001 ppm2      2.292
ASSI { 8621}
  (( segid "BrD " and resid 43   and name HN  ))
  (  segid "BrD " and resid 41   and name HG2%)
     4.200      4.200      1.300 peak  8621 weight  0.10000E+01 volume  0.33897E+02 ppm1      8.001 ppm2      1.887
ASSI { 8631}
  (( segid "BrD " and resid 43   and name HN  ))
  (  segid "BrD " and resid 38   and name HG1%)
     4.300      4.300      1.200 peak  8631 weight  0.10000E+01 volume  0.32108E+02 ppm1      8.002 ppm2      1.058
ASSI { 8641}
  (( segid "BrD " and resid 43   and name HN  ))
  (  segid "BrD " and resid 38   and name HG2%)
     3.900      3.800      1.600 peak  8641 weight  0.10000E+01 volume  0.57231E+02 ppm1      8.001 ppm2      0.778
ASSI { 8661}
  (( segid "BrD " and resid 111  and name HN  ))
  (( segid "BrD " and resid 112  and name HB1 ))
     3.800      3.600      1.700 peak  8661 weight  0.10000E+01 volume  0.66898E+02 ppm1      8.167 ppm2      2.659
ASSI { 8681}
  (( segid "BrD " and resid 111  and name HN  ))
  (  segid "BrD " and resid 110  and name HG2%)
     3.000      2.200      2.200 peak  8681 weight  0.10000E+01 volume  0.28506E+03 ppm1      8.169 ppm2      1.250
ASSI { 8691}
  (( segid "BrD " and resid 111  and name HN  ))
  (  segid "BrD " and resid 116  and name HD1%)
     3.400      2.900      2.100 peak  8691 weight  0.10000E+01 volume  0.11425E+03 ppm1      8.168 ppm2      1.396
ASSI { 8711}
  (( segid "BrD " and resid 58   and name HN  ))
  (( segid "BrD " and resid 37   and name HD1 ))
     3.700      3.400      1.800 peak  8711 weight  0.10000E+01 volume  0.73156E+02 ppm1     10.051 ppm2      4.255
ASSI { 8721}
  (( segid "BrD " and resid 58   and name HN  ))
  (( segid "BrD " and resid 59   and name HG2 ))
     5.500      5.500      0.000 peak  8721 weight  0.10000E+01 volume  0.48442E+00 ppm1     10.051 ppm2      3.087
ASSI { 8801}
  (( segid "BrD " and resid 58   and name HN  ))
  (  segid "BrD " and resid 54   and name HE% )
     4.600      4.600      0.900 peak  8801 weight  0.10000E+01 volume  0.21191E+02 ppm1     10.050 ppm2      2.534
ASSI { 8971}
  (( segid "BrD " and resid 112  and name HN  ))
  (  segid "BrD " and resid 110  and name HG2%)
     3.800      3.600      1.700 peak  8971 weight  0.10000E+01 volume  0.60828E+02 ppm1      8.669 ppm2      1.263
ASSI { 8991}
  (( segid "BrD " and resid 105  and name HN  ))
  (( segid "BrD " and resid 106  and name HB1 ))
     3.500      3.100      2.000 peak  8991 weight  0.10000E+01 volume  0.10888E+03 ppm1      8.487 ppm2      3.870
ASSI { 9041}
  (( segid "BrD " and resid 105  and name HN  ))
  (  segid "BrD " and resid 102  and name HD2%)
     3.700      3.400      1.800 peak  9041 weight  0.10000E+01 volume  0.76403E+02 ppm1      8.486 ppm2      1.320
OR { 9041}
  (( segid "BrD " and resid 105  and name HN  ))
  (  segid "BrD " and resid 102  and name HD1%)
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ASSI { 9051}
  (( segid "BrD " and resid 105  and name HN  ))
  (  segid "BrD " and resid 101  and name HG2%)
     3.900      3.800      1.600 peak  9051 weight  0.10000E+01 volume  0.50603E+02 ppm1      8.486 ppm2      1.602
ASSI { 9131}
  (( segid "BrD " and resid 21   and name HN  ))
  (( segid "BrD " and resid 21   and name HG12))
     3.200      2.600      2.300 peak  9131 weight  0.10000E+01 volume  0.17190E+03 ppm1      8.574 ppm2      1.620
OR { 9131}
  (( segid "BrD " and resid 21   and name HN  ))
  (  segid "BrD " and resid 21   and name HG2%)
ASSI { 9211}
  (( segid "BrD " and resid 106  and name HN  ))
  (  segid "BrD " and resid 102  and name HD2%)
     3.800      3.600      1.700 peak  9211 weight  0.10000E+01 volume  0.58744E+02 ppm1      9.740 ppm2      1.314
ASSI { 9221}
  (( segid "BrD " and resid 106  and name HN  ))
  (  segid "BrD " and resid 82   and name HE% )
     4.600      4.600      0.900 peak  9221 weight  0.10000E+01 volume  0.19539E+02 ppm1      9.740 ppm2      7.033
OR { 9221}
  (( segid "BrD " and resid 106  and name HN  ))
  (( segid "BrD " and resid 82   and name HZ  ))
ASSI { 9231}
  (( segid "BrD " and resid 84   and name HN  ))
  (( segid "BrD " and resid 80   and name HA  ))
     2.400      1.400      1.400 peak  9231 weight  0.10000E+01 volume  0.97933E+03 ppm1      9.464 ppm2      4.674
ASSI { 9261}
  (( segid "BrD " and resid 84   and name HN  ))
  (  segid "BrD " and resid 50   and name HD1%)
     4.700      4.700      0.800 peak  9261 weight  0.10000E+01 volume  0.17291E+02 ppm1      9.463 ppm2      1.136
ASSI { 9271}
  (( segid "BrD " and resid 84   and name HN  ))
  (( segid "BrD " and resid 50   and name HG2%)
     4.800      4.800      0.700 peak  9271 weight  0.10000E+01 volume  0.16063E+02 ppm1      9.464 ppm2      0.994
ASSI { 9361}
  (( segid "BrD " and resid 63   and name HN  ))
  (( segid "BrD " and resid 63   and name HB1 ))
     2.800      2.000      2.000 peak  9361 weight  0.10000E+01 volume  0.41354E+03 ppm1      9.456 ppm2      2.904
ASSI { 9411}
  (( segid "BrD " and resid 22   and name HN  ))
  (  segid "BrD " and resid 25   and name HG1%)
     3.600      3.200      1.900 peak  9411 weight  0.10000E+01 volume  0.92991E+02 ppm1      9.456 ppm2      1.797
ASSI { 9421}
  (( segid "BrD " and resid 22   and name HN  ))
  (  segid "BrD " and resid 21   and name HD1%)
     3.700      3.400      1.800 peak  9421 weight  0.10000E+01 volume  0.76602E+02 ppm1      9.456 ppm2      1.228
ASSI { 9431}
  (( segid "BrD " and resid 63   and name HN  ))
  (  segid "BrD " and resid 68   and name HD% )
     3.800      3.600      1.700 peak  9431 weight  0.10000E+01 volume  0.63643E+02 ppm1      9.456 ppm2      7.806
ASSI { 9481}
  (( segid "BrD " and resid 109  and name HN  ))
  (( segid "BrD " and resid 109  and name HD1 ))
     3.100      2.400      2.400 peak  9481 weight  0.10000E+01 volume  0.19915E+03 ppm1      8.556 ppm2      2.031
ASSI { 9521}
  (( segid "BrD " and resid 103  and name HN  ))
  (  segid "BrD " and resid 82   and name HE% )
     3.300      2.700      2.200 peak  9521 weight  0.10000E+01 volume  0.14688E+03 ppm1      8.695 ppm2      7.050
OR { 9521}
  (( segid "BrD " and resid 103  and name HN  ))
  (( segid "BrD " and resid 82   and name HZ  ))
ASSI { 9541}
  (( segid "BrD " and resid 113  and name HN  ))
  (( segid "BrD " and resid 111  and name HA  ))
     4.900      4.900      0.600 peak  9541 weight  0.10000E+01 volume  0.13131E+02 ppm1      8.696 ppm2      4.683
ASSI { 9611}
  (( segid "BrD " and resid 99   and name HN  ))
  (  segid "BrD " and resid 34   and name HE% )
     3.500      3.100      2.000 peak  9611 weight  0.10000E+01 volume  0.10701E+03 ppm1      8.936 ppm2      7.772
ASSI { 9671}
  (( segid "BrD " and resid 99   and name HN  ))
  (( segid "BrD " and resid 30   and name HB2 ))
     4.300      4.300      1.200 peak  9671 weight  0.10000E+01 volume  0.29603E+02 ppm1      8.936 ppm2      4.568
ASSI { 9681}
  (( segid "BrD " and resid 18   and name HN  ))
  (  segid "BrD " and resid 14   and name HD2%)
     3.600      3.200      1.900 peak  9681 weight  0.10000E+01 volume  0.80801E+02 ppm1      9.074 ppm2      1.390
OR { 9681}
  (( segid "BrD " and resid 18   and name HN  ))
  (  segid "BrD " and resid 14   and name HD1%)
ASSI { 9751}
  (( segid "BrD " and resid 64   and name HN  ))
  (( segid "BrD " and resid 63   and name HB2 ))
     2.400      1.400      1.400 peak  9751 weight  0.10000E+01 volume  0.10265E+04 ppm1      8.585 ppm2      2.532
ASSI { 9761}
  (( segid "BrD " and resid 64   and name HN  ))
  (  segid "BrD " and resid 63   and name HD2%)
     3.300      2.700      2.200 peak  9761 weight  0.10000E+01 volume  0.14024E+03 ppm1      8.585 ppm2      1.489
ASSI { 9811}
  (( segid "BrD " and resid 17   and name HN  ))
  (( segid "BrD " and resid 15   and name HB1 ))
     4.300      4.300      1.200 peak  9811 weight  0.10000E+01 volume  0.29691E+02 ppm1      8.669 ppm2      3.843
ASSI { 9851}
  (( segid "BrD " and resid 40   and name HN  ))
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   ( segid "BrD " and resid 41   and name HG2%)
     2.500     1.600     1.600 peak  9851 weight  0.10000E+01 volume  0.73405E+03 ppm1      8.669 ppm2      1.866
ASSI { 9871}
   (( segid "BrD " and resid 17   and name HN  ))
   ( segid "BrD " and resid 14   and name HD2%)
     4.000     4.000     1.500 peak  9871 weight  0.10000E+01 volume  0.46134E+02 ppm1      8.668 ppm2      1.379
OR { 9871}
   (( segid "BrD " and resid 17   and name HN  ))
   ( segid "BrD " and resid 14   and name HD1%)
ASSI { 9881}
   (( segid "BrD " and resid 17   and name HN  ))
   ( segid "BrD " and resid 18   and name HD2%)
     4.600     4.600     0.900 peak  9881 weight  0.10000E+01 volume  0.20602E+02 ppm1      8.669 ppm2      0.394
ASSI { 9911}
   (( segid "BrD " and resid 72   and name HN  ))
   (( segid "BrD " and resid 73   and name HB2 ))
     3.000     2.200     2.200 peak  9911 weight  0.10000E+01 volume  0.24469E+03 ppm1      8.858 ppm2      2.503
ASSI { 9951}
   (( segid "BrD " and resid 12   and name HN  ))
   (( segid "BrD " and resid 13   and name HA  ))
     3.800     3.600     1.700 peak  9951 weight  0.10000E+01 volume  0.59337E+02 ppm1      9.021 ppm2      4.770
ASSI { 9971}
   (( segid "BrD " and resid 12   and name HN  ))
   (( segid "BrD " and resid 15   and name HB2 ))
     4.100     4.100     1.400 peak  9971 weight  0.10000E+01 volume  0.38396E+02 ppm1      9.021 ppm2      3.618
ASSI { 9981}
   (( segid "BrD " and resid 12   and name HN  ))
   (( segid "BrD " and resid 11   and name HB1 ))
     3.200     2.600     2.300 peak  9981 weight  0.10000E+01 volume  0.16510E+03 ppm1      9.021 ppm2      2.971
ASSI { 9991}
   (( segid "BrD " and resid 12   and name HN  ))
   (( segid "BrD " and resid 11   and name HB2 ))
     3.300     2.700     2.200 peak  9991 weight  0.10000E+01 volume  0.13633E+03 ppm1      9.022 ppm2      2.611
OR { 9991}
   (( segid "BrD " and resid 12   and name HN  ))
   (( segid "BrD " and resid 11   and name HG1 ))
ASSI {10021}
   (( segid "BrD " and resid 25   and name HN  ))
   (( segid "BrD " and resid 26   and name HD1 ))
     3.700     3.400     1.800 peak 10021 weight  0.10000E+01 volume  0.71669E+02 ppm1      9.134 ppm2      2.092
ASSI {10031}
   (( segid "BrD " and resid 25   and name HN  ))
   ( segid "BrD " and resid 102  and name HD1%)
     3.800     3.600     1.700 peak 10031 weight  0.10000E+01 volume  0.60868E+02 ppm1      9.133 ppm2      1.295
OR {10031}
   (( segid "BrD " and resid 25   and name HN  ))
   ( segid "BrD " and resid 102  and name HD2%)
ASSI {10061}
   (( segid "BrD " and resid 24   and name HN  ))
   ( segid "BrD " and resid 25   and name HG1%)
     3.600     3.200     1.900 peak 10061 weight  0.10000E+01 volume  0.91063E+02 ppm1      8.657 ppm2      1.798
ASSI {10191}
   (( segid "BrD " and resid 16   and name HN  ))
   (( segid "BrD " and resid 18   and name HG  ))
     3.700     3.400     1.800 peak 10191 weight  0.10000E+01 volume  0.73953E+02 ppm1      8.792 ppm2      2.295
ASSI {10221}
   (( segid "BrD " and resid 76   and name HN  ))
   (( segid "BrD " and resid 74   and name HN  ))
     3.300     2.700     2.200 peak 10221 weight  0.10000E+01 volume  0.15827E+03 ppm1      8.611 ppm2      7.532
ASSI {10251}
   (( segid "BrD " and resid 75   and name HN  ))
   ( segid "BrD " and resid 18   and name HD1%)
     4.200     4.200     1.300 peak 10251 weight  0.10000E+01 volume  0.32785E+02 ppm1      9.105 ppm2      1.056
ASSI {10261}
   (( segid "BrD " and resid 75   and name HN  ))
   ( segid "BrD " and resid 76   and name HB% )
     3.400     2.900     2.100 peak 10261 weight  0.10000E+01 volume  0.13102E+03 ppm1      9.106 ppm2      2.099
ASSI {10291}
   (( segid "BrD " and resid 75   and name HN  ))
   ( segid "BrD " and resid 75   and name HE% )
     3.800     3.600     1.700 peak 10291 weight  0.10000E+01 volume  0.67546E+02 ppm1      9.108 ppm2      2.654
ASSI {10301}
   (( segid "BrD " and resid 75   and name HN  ))
   ( segid "BrD " and resid 18   and name HD2%)
     3.900     3.800     1.600 peak 10301 weight  0.10000E+01 volume  0.57563E+02 ppm1      9.106 ppm2      0.429
ASSI {10351}
   (( segid "BrD " and resid 95   and name HN  ))
   (( segid "BrD " and resid 93   and name HB1 ))
     2.900     2.100     2.100 peak 10351 weight  0.10000E+01 volume  0.35043E+03 ppm1      8.669 ppm2      5.018
ASSI {10401}
   (( segid "BrD " and resid 55   and name HN  ))
   (( segid "BrD " and resid 37   and name HB2 ))
     3.600     3.200     1.900 peak 10401 weight  0.10000E+01 volume  0.94850E+02 ppm1      7.996 ppm2      2.295
ASSI {10421}
   (( segid "BrD " and resid 55   and name HN  ))
   (( segid "BrD " and resid 37   and name HG2 ))
     2.700     1.800     1.800 peak 10421 weight  0.10000E+01 volume  0.46013E+03 ppm1      7.996 ppm2      2.578
ASSI {10441}
   (( segid "BrD " and resid 96   and name HN  ))
   (( segid "BrD " and resid 95   and name HB1 ))
     3.300     2.700     2.200 peak 10441 weight  0.10000E+01 volume  0.14200E+03 ppm1      7.988 ppm2      3.587
ASSI {10571}
   (( segid "BrD " and resid 80   and name HN  ))
   (( segid "BrD " and resid 79   and name HG1 ))
     2.400     1.400     1.400 peak 10571 weight  0.10000E+01 volume  0.10119E+04 ppm1      7.975 ppm2      3.105
ASSI {10581}
   (( segid "BrD " and resid 78   and name HN  ))
   (( segid "BrD " and resid 77   and name HB1 ))
     3.000     2.200     2.200 peak 10581 weight  0.10000E+01 volume  0.26376E+03 ppm1      7.974 ppm2      3.301
ASSI {10591}
   (( segid "BrD " and resid 55   and name HN  ))
   (( segid "BrD " and resid 58   and name HN  ))
     4.100     4.100     1.400 peak 10591 weight  0.10000E+01 volume  0.42990E+02 ppm1      7.972 ppm2     10.062
ASSI {10621}
   (( segid "BrD " and resid 56   and name HN  ))
   (( segid "BrD " and resid 34   and name HB1 ))
     3.700     3.400     1.800 peak 10621 weight  0.10000E+01 volume  0.69879E+02 ppm1      9.674 ppm2      4.100
ASSI {10641}
   (( segid "BrD " and resid 82   and name HN  ))
   (( segid "BrD " and resid 80   and name HB1 ))
     4.200     4.200     1.300 peak 10641 weight  0.10000E+01 volume  0.33240E+02 ppm1      6.981 ppm2      2.603
ASSI {10651}
   (( segid "BrD " and resid 82   and name HN  ))
   (( segid "BrD " and resid 84   and name HB2 ))
     4.300     4.300     1.200 peak 10651 weight  0.10000E+01 volume  0.31962E+02 ppm1      6.981 ppm2      3.230
ASSI {10661}
   (( segid "BrD " and resid 82   and name HN  ))
   ( segid "BrD " and resid 99   and name HB% )
     4.100     4.100     1.400 peak 10661 weight  0.10000E+01 volume  0.41756E+02 ppm1      6.981 ppm2      2.202
ASSI {10721}
   (( segid "BrD " and resid 81   and name HN  ))
   (( segid "BrD " and resid 77   and name HB1 ))
     3.900     3.800     1.600 peak 10721 weight  0.10000E+01 volume  0.54085E+02 ppm1      7.641 ppm2      3.310
ASSI {10751}
   (( segid "BrD " and resid 80   and name HN  ))
   (( segid "BrD " and resid 77   and name HB1 ))
     4.400     4.400     1.100 peak 10751 weight  0.10000E+01 volume  0.26321E+02 ppm1      8.005 ppm2      3.322
ASSI {10771}
   (( segid "BrD " and resid 80   and name HN  ))
   (( segid "BrD " and resid 81   and name HB  ))
     3.700     3.400     1.800 peak 10771 weight  0.10000E+01 volume  0.71103E+02 ppm1      8.006 ppm2      2.049
ASSI {10841}
   (( segid "BrD " and resid 79   and name HN  ))
   ( segid "BrD " and resid 76   and name HB% )
     3.500     3.100     2.000 peak 10841 weight  0.10000E+01 volume  0.10580E+03 ppm1      8.681 ppm2      2.096
ASSI {10881}
   (( segid "BrD " and resid 85   and name HN  ))
   ( segid "BrD " and resid 99   and name HB% )
     3.900     3.800     1.600 peak 10881 weight  0.10000E+01 volume  0.56660E+02 ppm1      7.515 ppm2      2.308
ASSI {10891}
   (( segid "BrD " and resid 85   and name HN  ))
   ( segid "BrD " and resid 81   and name HG2%)
     4.100     4.100     1.400 peak 10891 weight  0.10000E+01 volume  0.42261E+03 ppm1      7.522 ppm2      0.765
ASSI {10921}
   (( segid "BrD " and resid 86   and name HN  ))
   (( segid "BrD " and resid 87   and name HB1 ))
     3.800     3.600     1.700 peak 10921 weight  0.10000E+01 volume  0.59880E+02 ppm1      8.423 ppm2      2.779
OR {10921}
   (( segid "BrD " and resid 86   and name HN  ))
   (( segid "BrD " and resid 87   and name HG2 ))
ASSI {10931}
   (( segid "BrD " and resid 86   and name HN  ))
   (( segid "BrD " and resid 87   and name HB2 ))
     3.800     3.600     1.700 peak 10931 weight  0.10000E+01 volume  0.59561E+02 ppm1      8.423 ppm2      2.577
ASSI {10941}
   (( segid "BrD " and resid 86   and name HN  ))
   ( segid "BrD " and resid 99   and name HB% )
     3.600     3.200     1.900 peak 10941 weight  0.10000E+01 volume  0.93545E+02 ppm1      8.423 ppm2      2.210
ASSI {11001}
   (( segid "BrD " and resid 87   and name HN  ))
   ( segid "BrD " and resid 50   and name HD1%)
     3.800     3.600     1.700 peak 11001 weight  0.10000E+01 volume  0.61476E+02 ppm1      8.570 ppm2      1.148
ASSI {11021}
   (( segid "BrD " and resid 87   and name HN  ))
   (( segid "BrD " and resid 86   and name HG2 ))
     4.500     4.500     1.000 peak 11021 weight  0.10000E+01 volume  0.22088E+02 ppm1      8.571 ppm2      0.780
ASSI {11031}
   (( segid "BrD " and resid 88   and name HN  ))
   ( segid "BrD " and resid 50   and name HD1%)
     3.600     3.200     1.900 peak 11031 weight  0.10000E+01 volume  0.90228E+02 ppm1      8.354 ppm2      1.146
ASSI {11041}
   (( segid "BrD " and resid 88   and name HN  ))
   (( segid "BrD " and resid 84   and name HB2 ))
     4.000     4.000     1.500 peak 11041 weight  0.10000E+01 volume  0.46286E+02 ppm1      8.354 ppm2      3.299
ASSI {11051}
   (( segid "BrD " and resid 88   and name HN  ))
   (( segid "BrD " and resid 87   and name HG1 ))
     4.600     4.600     0.900 peak 11051 weight  0.10000E+01 volume  0.19886E+02 ppm1      8.354 ppm2      3.018
ASSI {11161}
   (( segid "BrD " and resid 93   and name HN  ))
   (( segid "BrD " and resid 91   and name HD2 ))
     3.700     3.400     1.800 peak 11161 weight  0.10000E+01 volume  0.78354E+02 ppm1      8.714 ppm2      6.410
ASSI {11171}
   (( segid "BrD " and resid 93   and name HN  ))
   (( segid "BrD " and resid 96   and name HB1 ))
     3.300     2.700     2.200 peak 11171 weight  0.10000E+01 volume  0.14983E+03 ppm1      8.714 ppm2      4.004
ASSI {11191}
   (( segid "BrD " and resid 30   and name HN  ))
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   (( segid "BrD " and resid 28   and name HB2 ))
      4.400      4.400      1.100 peak 11191 weight  0.10000E+01 volume  0.26154E+02 ppm1     12.276 ppm2      3.392
ASSI {11201}
   (( segid "BrD " and resid 30   and name HN  ))
   (( segid "BrD " and resid 28   and name HB1 ))
      3.300      2.700      2.200 peak 11201 weight  0.10000E+01 volume  0.18024E+03 ppm1     12.275 ppm2      3.594
ASSI {11211}
   (( segid "BrD " and resid 30   and name HN  ))
   (( segid "BrD " and resid 32   and name HN  ))
      3.600      3.200      1.900 peak 11211 weight  0.10000E+01 volume  0.82022E+02 ppm1     12.276 ppm2      7.741
ASSI {11241}
   (( segid "BrD " and resid 31   and name HN  ))
   (( segid "BrD " and resid 28   and name HB1 ))
      3.600      3.200      1.900 peak 11241 weight  0.10000E+01 volume  0.94685E+02 ppm1      8.480 ppm2      3.594
ASSI {11251}
   (( segid "BrD " and resid 31   and name HN  ))
   (( segid "BrD " and resid 28   and name HB2 ))
      3.800      3.600      1.700 peak 11251 weight  0.10000E+01 volume  0.64760E+02 ppm1      8.481 ppm2      3.389
ASSI {11361}
   (( segid "BrD " and resid 32   and name HN  ))
    ( segid "BrD " and resid 102  and name HD1% )
      4.500      4.500      1.000 peak 11361 weight  0.10000E+01 volume  0.23592E+02 ppm1      7.738 ppm2      1.310
ASSI {11391}
   (( segid "BrD " and resid 34   and name HN  ))
   (( segid "BrD " and resid 35   and name HG1 ))
      3.200      2.600      2.300 peak 11391 weight  0.10000E+01 volume  0.18521E+03 ppm1      8.182 ppm2      3.447
ASSI {11431}
   (( segid "BrD " and resid 34   and name HN  ))
    ( segid "BrD " and resid 31   and name HB% )
      2.900      2.100      2.100 peak 11431 weight  0.10000E+01 volume  0.29794E+03 ppm1      8.179 ppm2      2.301
ASSI {11441}
   (( segid "BrD " and resid 34   and name HN  ))
    ( segid "BrD " and resid 56   and name HD1% )
      3.400      2.900      2.100 peak 11441 weight  0.10000E+01 volume  0.12961E+03 ppm1      8.184 ppm2      1.527
ASSI {11451}
   (( segid "BrD " and resid 34   and name HN  ))
    ( segid "BrD " and resid 102  and name HD1% )
      3.600      3.200      1.900 peak 11451 weight  0.10000E+01 volume  0.84106E+02 ppm1      8.185 ppm2      1.305
ASSI {11521}
   (( segid "BrD " and resid 35   and name HN  ))
    ( segid "BrD " and resid 56   and name HD1% )
      4.500      4.500      1.000 peak 11521 weight  0.10000E+01 volume  0.22012E+02 ppm1      7.734 ppm2      1.553
ASSI {11561}
   (( segid "BrD " and resid 36   and name HN  ))
   (( segid "BrD " and resid 57   and name HB1 ))
      3.400      2.900      2.100 peak 11561 weight  0.10000E+01 volume  0.11642E+03 ppm1      8.308 ppm2      2.953
ASSI {11571}
   (( segid "BrD " and resid 66   and name HN  ))
    ( segid "BrD " and resid 63   and name HD1% )
      4.200      4.200      1.300 peak 11571 weight  0.10000E+01 volume  0.34773E+02 ppm1      8.763 ppm2      1.640
ASSI {11601}
   (( segid "BrD " and resid 67   and name HN  ))
    ( segid "BrD " and resid 68   and name HD% )
      4.400      4.400      1.100 peak 11601 weight  0.10000E+01 volume  0.26280E+02 ppm1      8.832 ppm2      7.780
ASSI {11651}
   (( segid "BrD " and resid 68   and name HN  ))
   (( segid "BrD " and resid 69   and name HB  ))
      3.700      3.400      1.800 peak 11651 weight  0.10000E+01 volume  0.74566E+02 ppm1      8.626 ppm2      2.947
ASSI {11661}
   (( segid "BrD " and resid 68   and name HN  ))
    ( segid "BrD " and resid 18   and name HD1% )
      5.500      5.500      0.000 peak 11661 weight  0.10000E+01 volume  0.40212E+01 ppm1      8.626 ppm2      1.090
ASSI {11731}
   (( segid "BrD " and resid 70   and name HN  ))
   (( segid "BrD " and resid 68   and name HB1 ))
      3.600      3.200      1.900 peak 11731 weight  0.10000E+01 volume  0.91804E+02 ppm1      8.040 ppm2      3.689
ASSI {11741}
   (( segid "BrD " and resid 70   and name HN  ))
   (( segid "BrD " and resid 74   and name HB1 ))
      3.400      2.900      2.100 peak 11741 weight  0.10000E+01 volume  0.13333E+03 ppm1      8.039 ppm2      3.544
ASSI {11771}
   (( segid "BrD " and resid 70   and name HN  ))
   (( segid "BrD " and resid 73   and name HB2 ))
      3.700      3.400      1.800 peak 11771 weight  0.10000E+01 volume  0.79558E+02 ppm1      8.040 ppm2      2.491
ASSI {11841}
   (( segid "BrD " and resid 73   and name HN  ))
   (( segid "BrD " and resid 70   and name HB2 ))
      3.200      2.600      2.300 peak 11841 weight  0.10000E+01 volume  0.16883E+03 ppm1      8.047 ppm2      4.361
ASSI {11891}
   (( segid "BrD " and resid 74   and name HN  ))
   (( segid "BrD " and resid 75   and name HB2 ))
      4.700      4.700      0.800 peak 11891 weight  0.10000E+01 volume  0.18157E+02 ppm1      7.536 ppm2      2.851
ASSI {11911}
   (( segid "BrD " and resid 74   and name HN  ))
    ( segid "BrD " and resid 76   and name HB% )
      4.400      4.400      1.100 peak 11911 weight  0.10000E+01 volume  0.27875E+02 ppm1      7.536 ppm2      2.088
ASSI {12031}
   (( segid "BrD " and resid 99   and name HN  ))
   (( segid "BrD " and resid 100  and name HB2 ))
      3.800      3.600      1.700 peak 12031 weight  0.10000E+01 volume  0.61845E+02 ppm1      8.936 ppm2      3.439
ASSI {12041}
   (( segid "BrD " and resid 99   and name HN  ))
   (( segid "BrD " and resid 97   and name HB1 ))
      3.400      2.900      2.100 peak 12041 weight  0.10000E+01 volume  0.12562E+03 ppm1      8.936 ppm2      2.721
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ASSI {12061}
   (( segid "BrD " and resid 100  and name HN  ))
   (( segid "BrD " and resid 101  and name HA  ))
      4.000      4.000      1.500 peak 12061 weight  0.10000E+01 volume  0.47923E+02 ppm1      8.669 ppm2      4.288
ASSI {12091}
   (( segid "BrD " and resid 100  and name HN  ))
   (( segid "BrD " and resid 101  and name HG11))
      4.100      4.100      1.400 peak 12091 weight  0.10000E+01 volume  0.39843E+02 ppm1      8.669 ppm2      2.519
OR {12091}
   (( segid "BrD " and resid 100  and name HN  ))
   (( segid "BrD " and resid 101  and name HB  ))
ASSI {12151}
   (( segid "BrD " and resid 101  and name HN  ))
   (( segid "BrD " and resid 104  and name HD1 ))
      3.500      3.100      2.000 peak 12151 weight  0.10000E+01 volume  0.11138E+03 ppm1      8.513 ppm2      2.282
ASSI {12221}
   (( segid "BrD " and resid 107  and name HN  ))
    ( segid "BrD " and resid 106  and name HD% )
      3.300      2.700      2.200 peak 12221 weight  0.10000E+01 volume  0.14273E+03 ppm1      8.981 ppm2      7.515
ASSI {12241}
   (( segid "BrD " and resid 107  and name HN  ))
   (( segid "BrD " and resid 103  and name HG2 ))
      3.400      2.900      2.100 peak 12241 weight  0.10000E+01 volume  0.11969E+03 ppm1      8.980 ppm2      2.547
ASSI {12271}
   (( segid "BrD " and resid 107  and name HN  ))
   (( segid "BrD " and resid 110  and name HG12))
      4.000      4.000      1.500 peak 12271 weight  0.10000E+01 volume  0.48486E+02 ppm1      8.980 ppm2      1.678
ASSI {12291}
   (( segid "BrD " and resid 108  and name HN  ))
   (( segid "BrD " and resid 109  and name HB2 ))
      5.500      5.500      0.000 peak 12291 weight  0.10000E+01 volume  0.20202E+00 ppm1      8.522 ppm2      2.195
ASSI {12411}
   (( segid "BrD " and resid 113  and name HN  ))
    ( segid "BrD " and resid 17   and name HG2% )
      4.300      4.300      1.200 peak 12411 weight  0.10000E+01 volume  0.28750E+02 ppm1      8.218 ppm2      1.728
ASSI {12431}
   (( segid "BrD " and resid 113  and name HN  ))
    ( segid "BrD " and resid 110  and name HG2% )
      3.400      2.900      2.100 peak 12431 weight  0.10000E+01 volume  0.12771E+03 ppm1      8.218 ppm2      1.275
ASSI {12441}
   (( segid "BrD " and resid 115  and name HN  ))
    ( segid "BrD " and resid 113  and name HB% )
      3.400      2.900      2.100 peak 12441 weight  0.10000E+01 volume  0.11633E+03 ppm1      8.355 ppm2      1.969
ASSI {12451}
   (( segid "BrD " and resid 115  and name HN  ))
   (( segid "BrD " and resid 116  and name HG12))
      5.500      5.500      0.000 peak 12451 weight  0.10000E+01 volume  0.47664E+01 ppm1      8.355 ppm2      1.558
ASSI {12461}
   (( segid "BrD " and resid 115  and name HN  ))
    ( segid "BrD " and resid 110  and name HD1% )
      4.400      4.400      1.100 peak 12461 weight  0.10000E+01 volume  0.26420E+02 ppm1      8.356 ppm2      1.163
ASSI {12471}
   (( segid "BrD " and resid 115  and name HN  ))
   (( segid "BrD " and resid 110  and name HB  ))
      3.700      3.400      1.800 peak 12471 weight  0.10000E+01 volume  0.76081E+02 ppm1      8.355 ppm2      2.346
ASSI {12481}
   (( segid "BrD " and resid 117  and name HN  ))
   (( segid "BrD " and resid 116  and name HG12))
      4.700      4.700      0.800 peak 12481 weight  0.10000E+01 volume  0.17262E+02 ppm1      8.883 ppm2      1.544
ASSI {12491}
   (( segid "BrD " and resid 116  and name HN  ))
    ( segid "BrD " and resid 110  and name HG2% )
      3.200      2.600      2.300 peak 12491 weight  0.10000E+01 volume  0.16590E+03 ppm1      8.083 ppm2      1.277
ASSI {12521}
   (( segid "BrD " and resid 116  and name HN  ))
    ( segid "BrD " and resid 110  and name HD1% )
      3.200      2.600      2.300 peak 12521 weight  0.10000E+01 volume  0.17496E+03 ppm1      8.086 ppm2      1.156
ASSI {12591}
   (( segid "BrD " and resid 47   and name HN  ))
   (( segid "BrD " and resid 48   and name HG2 ))
      4.200      4.200      1.300 peak 12591 weight  0.10000E+01 volume  0.33544E+02 ppm1      8.832 ppm2      2.861
ASSI {12611}
   (( segid "BrD " and resid 47   and name HN  ))
    ( segid "BrD " and resid 43   and name HB% )
      3.800      3.600      1.700 peak 12611 weight  0.10000E+01 volume  0.60519E+02 ppm1      8.832 ppm2      1.700
ASSI {12621}
   (( segid "BrD " and resid 49   and name HN  ))
   (( segid "BrD " and resid 50   and name HB  ))
      3.600      3.200      1.900 peak 12621 weight  0.10000E+01 volume  0.90984E+02 ppm1      7.762 ppm2      1.797
ASSI {12701}
   (( segid "BrD " and resid 52   and name HN  ))
   (( segid "BrD " and resid 53   and name HG1 ))
      3.900      3.800      1.600 peak 12701 weight  0.10000E+01 volume  0.53690E+02 ppm1      9.004 ppm2      2.820
OR {12701}
   (( segid "BrD " and resid 52   and name HN  ))
   (( segid "BrD " and resid 53   and name HB1 ))
ASSI {12741}
   (( segid "BrD " and resid 42   and name HN  ))
   (( segid "BrD " and resid 39   and name HB1 ))
      3.100      2.400      2.400 peak 12741 weight  0.10000E+01 volume  0.21408E+03 ppm1      7.820 ppm2      2.491
ASSI {12751}
   (( segid "BrD " and resid 42   and name HN  ))
   (( segid "BrD " and resid 39   and name HD1 ))
      3.000      2.200      2.200 peak 12751 weight  0.10000E+01 volume  0.25898E+03 ppm1      7.821 ppm2      2.386
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ASSI (12761)
  (( segid "BrD " and resid 42   and name HN  ))
  ( segid "BrD " and resid 43   and name HB% )
    3.500     3.100     2.000 peak 12761 weight  0.10000E+01 volume  0.10310E+03 ppm1      7.820 ppm2      1.706
ASSI (12851)
  (( segid "BrD " and resid 20   and name HN  ))
  (( segid "BrD " and resid 19   and name HD1 ))
    3.600     3.200     1.900 peak 12851 weight  0.10000E+01 volume  0.82185E+02 ppm1      8.145 ppm2      2.189
ASSI (12881)
  (( segid "BrD " and resid 20   and name HN  ))
  (( segid "BrD " and resid 21   and name HG12))
    3.900     3.800     1.600 peak 12881 weight  0.10000E+01 volume  0.55288E+02 ppm1      8.147 ppm2      1.639
OR (12881)
  (( segid "BrD " and resid 20   and name HN  ))
  ( segid "BrD " and resid 21   and name HG2%)
ASSI (12891)
  (( segid "BrD " and resid 20   and name HN  ))
  ( segid "BrD " and resid 63   and name HD2%)
    3.500     3.100     2.000 peak 12891 weight  0.10000E+01 volume  0.11141E+03 ppm1      8.146 ppm2      1.480
ASSI (12901)
  (( segid "BrD " and resid 20   and name HN  ))
  ( segid "BrD " and resid 17   and name HG2%)
    3.900     3.800     1.600 peak 12901 weight  0.10000E+01 volume  0.83573E+02 ppm1      8.146 ppm2      1.762
ASSI (12991)
  (( segid "BrD " and resid 23   and name HN  ))
  (( segid "BrD " and resid 20   and name HN  ))
    3.800     3.600     1.700 peak 12991 weight  0.10000E+01 volume  0.61946E+02 ppm1      9.119 ppm2      8.121
ASSI (13021)
  (( segid "BrD " and resid 26   and name HN  ))
  (( segid "BrD " and resid 28   and name HB2 ))
    4.200     4.200     1.300 peak 13021 weight  0.10000E+01 volume  0.33211E+02 ppm1      9.196 ppm2      3.393
ASSI (13031)
  (( segid "BrD " and resid 26   and name HN  ))
  (( segid "BrD " and resid 35   and name HG1 ))
    4.500     4.500     1.000 peak 13031 weight  0.10000E+01 volume  0.21672E+02 ppm1      9.195 ppm2      3.493
ASSI (13041)
  (( segid "BrD " and resid 26   and name HN  ))
  ( segid "BrD " and resid 56   and name HD2%)
    4.100     4.100     1.400 peak 13041 weight  0.10000E+01 volume  0.41596E+02 ppm1      9.196 ppm2      1.250
ASSI (13061)
  (( segid "BrD " and resid 27   and name HN  ))
  (( segid "BrD " and resid 26   and name HG1 ))
    3.800     3.600     1.700 peak 13061 weight  0.10000E+01 volume  0.66585E+02 ppm1      8.169 ppm2      1.596
ASSI (13091)
  (( segid "BrD " and resid 27   and name HN  ))
  ( segid "BrD " and resid 35   and name HE% )
    3.600     3.200     1.900 peak 13091 weight  0.10000E+01 volume  0.88198E+02 ppm1      8.169 ppm2      2.809
ASSI (13111)
  (( segid "BrD " and resid 59   and name HN  ))
  ( segid "BrD " and resid 59   and name HE% )
    3.300     2.700     2.200 peak 13111 weight  0.10000E+01 volume  0.15860E+03 ppm1      8.498 ppm2      1.864
ASSI (13131)
  (( segid "BrD " and resid 59   and name HN  ))
  ( segid "BrD " and resid 56   and name HD2%)
    4.300     4.300     1.200 peak 13131 weight  0.10000E+01 volume  0.28520E+02 ppm1      8.499 ppm2      1.239
ASSI (13161)
  (( segid "BrD " and resid 60   and name HN  ))
  (( segid "BrD " and resid 59   and name HG1 ))
    3.600     3.200     1.900 peak 13161 weight  0.10000E+01 volume  0.93397E+02 ppm1      8.565 ppm2      3.213
ASSI (13221)
  (( segid "BrD " and resid 32   and name HE1 ))
  (( segid "BrD " and resid 32   and name HD1 ))
    2.300     1.300     1.300 peak 13221 weight  0.10000E+01 volume  0.12506E+04 ppm1     11.082 ppm2      8.475
ASSI (13231)
  (( segid "BrD " and resid 32   and name HE1 ))
  (( segid "BrD " and resid 32   and name HN  ))
    3.200     2.600     2.300 peak 13231 weight  0.10000E+01 volume  0.18835E+03 ppm1     11.082 ppm2      7.742
OR (13231)
  (( segid "BrD " and resid 32   and name HE1 ))
  (( segid "BrD " and resid 32   and name HH2 ))
ASSI (13241)
  (( segid "BrD " and resid 32   and name HE1 ))
  (( segid "BrD " and resid 32   and name HZ2 ))
    2.500     1.600     1.600 peak 13241 weight  0.10000E+01 volume  0.70734E+03 ppm1     11.082 ppm2      7.984
ASSI (13251)
  (( segid "BrD " and resid 32   and name HE1 ))
  (( segid "BrD " and resid 30   and name HA  ))
    3.100     2.400     2.400 peak 13251 weight  0.10000E+01 volume  0.32949E+03 ppm1     11.082 ppm2      5.450
ASSI (13301)
  (( segid "BrD " and resid 76   and name HN  ))
  (( segid "BrD " and resid 77   and name HA  ))
    4.200     4.200     1.300 peak 13301 weight  0.10000E+01 volume  0.33586E+02 ppm1      8.610 ppm2      4.967
ASSI (13311)
  (( segid "BrD " and resid 76   and name HN  ))
  (( segid "BrD " and resid 77   and name HB1 ))
    4.100     4.100     1.400 peak 13311 weight  0.10000E+01 volume  0.37785E+02 ppm1      8.613 ppm2      3.344
ASSI (13651)
  (( segid "BrD " and resid 56   and name HN  ))
  ( segid "BrD " and resid 61   and name HG1%)
    4.100     4.100     1.400 peak 13651 weight  0.10000E+01 volume  0.38100E+02 ppm1      9.680 ppm2      1.077
ASSI (13661)
  (( segid "BrD " and resid 56   and name HN  ))
  ( segid "BrD " and resid 61   and name HG2%)
    4.200     4.200     1.300 peak 13661 weight  0.10000E+01 volume  0.33875E+02 ppm1      9.681 ppm2      0.743
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ASSI (13681)
  (( segid "BrD " and resid 74   and name HN  ))
  ( segid "BrD " and resid 14   and name HD1%)
    4.700     4.700     0.800 peak 13681 weight  0.10000E+01 volume  0.17399E+02 ppm1      7.536 ppm2      1.405
OR (13681)
  (( segid "BrD " and resid 74   and name HN  ))
  ( segid "BrD " and resid 14   and name HD2%)
ASSI (13721)
  (( segid "BrD " and resid 16   and name HN  ))
  (( segid "BrD " and resid 17   and name HB  ))
    4.400     4.400     1.100 peak 13721 weight  0.10000E+01 volume  0.26713E+02 ppm1      8.794 ppm2      4.874
ASSI (13751)
  (( segid "BrD " and resid 74   and name HN  ))
  (( segid "BrD " and resid 68   and name HA  ))
    5.300     5.300     0.200 peak 13751 weight  0.10000E+01 volume  0.81254E+01 ppm1      7.537 ppm2      5.140
ASSI (13881)
  (( segid "BrD " and resid 46   and name HN  ))
  ( segid "BrD " and resid 38   and name HG1%)
    4.600     4.600     0.900 peak 13881 weight  0.10000E+01 volume  0.18836E+02 ppm1      8.562 ppm2      1.082
ASSI (13891)
  (( segid "BrD " and resid 62   and name HN  ))
  (( segid "BrD " and resid 67   and name HB1 ))
    4.100     4.100     1.400 peak 13891 weight  0.10000E+01 volume  0.40043E+02 ppm1      8.998 ppm2      3.557
ASSI (13931)
  (( segid "BrD " and resid 116  and name HN  ))
  ( segid "BrD " and resid 75   and name HE% )
    5.000     5.000     0.500 peak 13931 weight  0.10000E+01 volume  0.12168E+02 ppm1      8.086 ppm2      2.648
ASSI (13941)
  (( segid "BrD " and resid 115  and name HN  ))
  (( segid "BrD " and resid 110  and name HA  ))
    4.100     4.100     1.400 peak 13941 weight  0.10000E+01 volume  0.38338E+02 ppm1      8.355 ppm2      4.419
ASSI (13951)
  (( segid "BrD " and resid 114  and name HN  ))
  (( segid "BrD " and resid 112  and name HN  ))
    4.000     4.000     1.500 peak 13951 weight  0.10000E+01 volume  0.49230E+02 ppm1      8.375 ppm2      8.642
ASSI (13961)
  (( segid "BrD " and resid 114  and name HN  ))
  (( segid "BrD " and resid 112  and name HB1 ))
    5.200     5.200     0.300 peak 13961 weight  0.10000E+01 volume  0.99997E+01 ppm1      8.377 ppm2      2.665
ASSI (14001)
  (( segid "BrD " and resid 108  and name HN  ))
  (( segid "BrD " and resid 106  and name HN  ))
    4.900     4.900     0.600 peak 14001 weight  0.10000E+01 volume  0.12922E+02 ppm1      8.529 ppm2      9.745
ASSI (14021)
  (( segid "BrD " and resid 108  and name HN  ))
  (( segid "BrD " and resid 104  and name HA  ))
    2.700     1.800     1.800 peak 14021 weight  0.10000E+01 volume  0.54819E+03 ppm1      8.526 ppm2      4.663
ASSI (14031)
  (( segid "BrD " and resid 108  and name HN  ))
  (( segid "BrD " and resid 110  and name HG12))
    5.200     5.200     0.300 peak 14031 weight  0.10000E+01 volume  0.95149E+01 ppm1      8.521 ppm2      1.696
ASSI (14051)
  (( segid "BrD " and resid 107  and name HN  ))
  (( segid "BrD " and resid 108  and name HA  ))
    4.500     4.500     1.000 peak 14051 weight  0.10000E+01 volume  0.23253E+02 ppm1      8.980 ppm2      4.798
ASSI (14081)
  (( segid "BrD " and resid 106  and name HN  ))
  ( segid "BrD " and resid 21   and name HG2%)
    4.600     4.600     0.900 peak 14081 weight  0.10000E+01 volume  0.21267E+02 ppm1      9.740 ppm2      1.640
ASSI (14091)
  (( segid "BrD " and resid 105  and name HN  ))
  (( segid "BrD " and resid 106  and name HA  ))
    4.500     4.500     1.000 peak 14091 weight  0.10000E+01 volume  0.22190E+02 ppm1      8.487 ppm2      4.568
ASSI (14101)
  (( segid "BrD " and resid 105  and name HN  ))
  (( segid "BrD " and resid 103  and name HB2 ))
    5.000     5.000     0.500 peak 14101 weight  0.10000E+01 volume  0.11917E+02 ppm1      8.487 ppm2      1.881
ASSI (14181)
  (( segid "BrD " and resid 100  and name HN  ))
  (( segid "BrD " and resid 34   and name HZ  ))
    4.700     4.700     0.800 peak 14181 weight  0.10000E+01 volume  0.18067E+02 ppm1      8.675 ppm2      7.907
ASSI (14211)
  (( segid "BrD " and resid 100  and name HN  ))
  (( segid "BrD " and resid 97   and name HB1 ))
    4.400     4.400     1.100 peak 14211 weight  0.10000E+01 volume  0.25437E+02 ppm1      8.669 ppm2      2.715
ASSI (14231)
  (( segid "BrD " and resid 99   and name HN  ))
  (( segid "BrD " and resid 101  and name HN  ))
    4.300     4.300     1.200 peak 14231 weight  0.10000E+01 volume  0.28380E+02 ppm1      8.936 ppm2      8.500
ASSI (14261)
  (( segid "BrD " and resid 99   and name HN  ))
  (( segid "BrD " and resid 33   and name HG1 ))
    5.500     5.500     0.000 peak 14261 weight  0.10000E+01 volume  0.32802E+01 ppm1      8.936 ppm2      0.866
ASSI (14271)
  (( segid "BrD " and resid 98   and name HN  ))
  (( segid "BrD " and resid 101  and name HN  ))
    4.400     4.400     1.100 peak 14271 weight  0.10000E+01 volume  0.25780E+02 ppm1      9.125 ppm2      8.916
ASSI (14291)
  (( segid "BrD " and resid 97   and name HN  ))
  (( segid "BrD " and resid 93   and name HB1 ))
    5.500     5.500     0.000 peak 14291 weight  0.10000E+01 volume  0.62831E+01 ppm1      8.677 ppm2      5.016
OR (14291)
  (( segid "BrD " and resid 97   and name HN  ))
  (( segid "BrD " and resid 93   and name HA  ))
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ASSI (14321)
  (( segid "BrD " and resid 95   and name HN  ))
  (( segid "BrD " and resid 32   and name HN2 ))
    3.700     3.400     1.800 peak 14321 weight  0.10000E+01 volume  0.76926E+02 ppm1     8.669 ppm2     7.739
ASSI (14331)
  (( segid "BrD " and resid 93   and name HN  ))
  (( segid "BrD " and resid 96   and name HN  ))
    4.500     4.500     1.000 peak 14331 weight  0.10000E+01 volume  0.22598E+02 ppm1     8.713 ppm2     7.963
ASSI (14351)
  (( segid "BrD " and resid 93   and name HN  ))
  (( segid "BrD " and resid 95   and name HB1 ))
    4.600     4.600     0.900 peak 14351 weight  0.10000E+01 volume  0.20643E+02 ppm1     8.714 ppm2     3.617
ASSI (14381)
  (( segid "BrD " and resid 87   and name HN  ))
  (( segid "BrD " and resid 89   and name HD21))
    3.900     3.800     1.600 peak 14381 weight  0.10000E+01 volume  0.54969E+02 ppm1     8.568 ppm2     8.959
ASSI (14391)
  (( segid "BrD " and resid 87   and name HN  ))
  (( segid "BrD " and resid 89   and name HN  ))
    3.600     3.200     1.900 peak 14391 weight  0.10000E+01 volume  0.81305E+02 ppm1     8.568 ppm2     8.838
ASSI (14431)
  (( segid "BrD " and resid 85   and name HN  ))
  (( segid "BrD " and resid 87   and name HN  ))
    4.100     4.100     1.400 peak 14431 weight  0.10000E+01 volume  0.42435E+02 ppm1     7.516 ppm2     8.557
ASSI (14471)
  (( segid "BrD " and resid 82   and name HN  ))
  (( segid "BrD " and resid 80   and name HN  ))
    4.800     4.800     0.700 peak 14471 weight  0.10000E+01 volume  0.16164E+02 ppm1     6.979 ppm2     7.979
ASSI (14521)
  (( segid "BrD " and resid 79   and name HN  ))
  (( segid "BrD " and resid 77   and name HA  ))
    4.800     4.800     0.700 peak 14521 weight  0.10000E+01 volume  0.15931E+02 ppm1     8.679 ppm2     4.968
ASSI (14531)
  (( segid "BrD " and resid 79   and name HN  ))
  (  segid "BrD " and resid 59   and name HE% )
    4.000     4.000     1.500 peak 14531 weight  0.10000E+01 volume  0.45701E+02 ppm1     8.680 ppm2     1.876
ASSI (14561)
  (( segid "BrD " and resid 76   and name HN  ))
  (( segid "BrD " and resid 74   and name HA  ))
    4.300     4.300     1.200 peak 14561 weight  0.10000E+01 volume  0.31541E+02 ppm1     8.611 ppm2     4.361
ASSI (14601)
  (( segid "BrD " and resid 72   and name HN  ))
  (( segid "BrD " and resid 75   and name HB2 ))
    4.600     4.600     0.900 peak 14601 weight  0.10000E+01 volume  0.21235E+02 ppm1     8.659 ppm2     2.805
ASSI (14611)
  (( segid "BrD " and resid 72   and name HN  ))
  (( segid "BrD " and resid 9    and name HB1 ))
    3.600     3.200     1.900 peak 14611 weight  0.10000E+01 volume  0.90159E+02 ppm1     8.859 ppm2     2.443
ASSI (14661)
  (( segid "BrD " and resid 64   and name HN  ))
  (( segid "BrD " and resid 62   and name HN  ))
    4.100     4.100     1.400 peak 14661 weight  0.10000E+01 volume  0.40125E+02 ppm1     8.585 ppm2     8.966
ASSI (14681)
  (( segid "BrD " and resid 64   and name HN  ))
  (( segid "BrD " and resid 65   and name HB2 ))
    4.800     4.800     0.700 peak 14681 weight  0.10000E+01 volume  0.16509E+02 ppm1     8.584 ppm2     3.383
ASSI (14711)
  (( segid "BrD " and resid 63   and name HN  ))
  (  segid "BrD " and resid 74   and name HD% )
    4.600     4.600     0.900 peak 14711 weight  0.10000E+01 volume  0.18909E+02 ppm1     9.471 ppm2     7.007
ASSI (14741)
  (( segid "BrD " and resid 62   and name HN  ))
  (( segid "BrD " and resid 61   and name HN  ))
    2.600     1.700     1.700 peak 14741 weight  0.10000E+01 volume  0.63142E+03 ppm1     8.997 ppm2     8.742
ASSI (14771)
  (( segid "BrD " and resid 62   and name HN  ))
  (( segid "BrD " and resid 65   and name HB2 ))
    4.200     4.200     1.300 peak 14771 weight  0.10000E+01 volume  0.33744E+02 ppm1     8.999 ppm2     3.355
ASSI (14841)
  (( segid "BrD " and resid 57   and name HN  ))
  (( segid "BrD " and resid 35   and name HA  ))
    3.200     2.600     2.300 peak 14841 weight  0.10000E+01 volume  0.16187E+03 ppm1     9.359 ppm2     4.904
ASSI (14861)
  (( segid "BrD " and resid 55   and name HN  ))
  (( segid "BrD " and resid 59   and name HN  ))
    3.900     3.800     1.600 peak 14861 weight  0.10000E+01 volume  0.53302E+02 ppm1     7.974 ppm2     8.498
ASSI (14891)
  (( segid "BrD " and resid 54   and name HN  ))
  (( segid "BrD " and resid 84   and name HB1 ))
    4.600     4.600     0.900 peak 14891 weight  0.10000E+01 volume  0.21172E+02 ppm1     9.037 ppm2     3.597
ASSI (14981)
  (( segid "BrD " and resid 48   and name HN  ))
  (( segid "BrD " and resid 46   and name HB2 ))
    4.300     4.300     1.200 peak 14981 weight  0.10000E+01 volume  0.30250E+02 ppm1     8.306 ppm2     3.090
ASSI (14991)
  (( segid "BrD " and resid 48   and name HN  ))
  (  segid "BrD " and resid 49   and name HG1%)
    3.700     3.400     1.800 peak 14991 weight  0.10000E+01 volume  0.71559E+02 ppm1     8.305 ppm2     1.639
ASSI (15001)
  (( segid "BrD " and resid 92   and name HN  ))
  (( segid "BrD " and resid 89   and name HD22))
    4.900     4.900     0.600 peak 15001 weight  0.10000E+01 volume  0.14588E+02 ppm1     8.832 ppm2     8.433
ASSI (15011)
  (( segid "BrD " and resid 47   and name HN  ))
  (( segid "BrD " and resid 49   and name HN  ))
    4.000     4.000     1.500 peak 15011 weight  0.10000E+01 volume  0.44203E+02 ppm1     8.832 ppm2     7.759
ASSI (15041)
  (( segid "BrD " and resid 43   and name HN  ))
  (( segid "BrD " and resid 42   and name HG1 ))
    4.000     4.000     1.500 peak 15041 weight  0.10000E+01 volume  0.44922E+02 ppm1     8.000 ppm2     2.889
ASSI (15071)
  (( segid "BrD " and resid 35   and name HN  ))
  (( segid "BrD " and resid 33   and name HA  ))
    4.300     4.300     1.200 peak 15071 weight  0.10000E+01 volume  0.32086E+02 ppm1     7.735 ppm2     4.346
ASSI (15081)
  (( segid "BrD " and resid 35   and name HN  ))
  (( segid "BrD " and resid 34   and name HB1 ))
    3.800     3.600     1.700 peak 15081 weight  0.10000E+01 volume  0.61308E+02 ppm1     7.734 ppm2     4.079
ASSI (15111)
  (( segid "BrD " and resid 34   and name HN  ))
  (  segid "BrD " and resid 81   and name HG2%)
    4.700     4.700     0.800 peak 15111 weight  0.10000E+01 volume  0.17971E+02 ppm1     8.178 ppm2     0.756
ASSI (15131)
  (( segid "BrD " and resid 32   and name HN  ))
  (( segid "BrD " and resid 33   and name HG1 ))
    5.400     5.400     0.100 peak 15131 weight  0.10000E+01 volume  0.80091E+01 ppm1     7.739 ppm2     0.859
ASSI (15141)
  (( segid "BrD " and resid 31   and name HN  ))
  (( segid "BrD " and resid 28   and name HN  ))
    3.200     2.600     2.300 peak 15141 weight  0.10000E+01 volume  0.16166E+03 ppm1     8.480 ppm2     8.159
OR (15141)
  (( segid "BrD " and resid 31   and name HN  ))
  (( segid "BrD " and resid 28   and name HE1 ))
ASSI (15161)
  (( segid "BrD " and resid 30   and name HN  ))
  (  segid "BrD " and resid 31   and name HB% )
    3.800     3.600     1.700 peak 15161 weight  0.10000E+01 volume  0.65201E+02 ppm1     12.276 ppm2    2.299
ASSI (15171)
  (( segid "BrD " and resid 30   and name HN  ))
  (  segid "BrD " and resid 102  and name HD1%)
    3.900     3.800     1.600 peak 15171 weight  0.10000E+01 volume  0.51602E+02 ppm1     12.275 ppm2    1.315
ASSI (15191)
  (( segid "BrD " and resid 29   and name HN  ))
  (( segid "BrD " and resid 31   and name HN  ))
    5.000     5.000     0.500 peak 15191 weight  0.10000E+01 volume  0.12673E+02 ppm1     9.152 ppm2     8.470
ASSI (15201)
  (( segid "BrD " and resid 29   and name HN  ))
  (( segid "BrD " and resid 30   and name HB1 ))
    4.300     4.300     1.200 peak 15201 weight  0.10000E+01 volume  0.29023E+02 ppm1     9.151 ppm2     4.941
ASSI (15211)
  (( segid "BrD " and resid 29   and name HN  ))
  (  segid "BrD " and resid 101  and name HD1%)
    5.000     5.000     0.500 peak 15211 weight  0.10000E+01 volume  0.12825E+02 ppm1     9.153 ppm2     1.558
ASSI (15261)
  (( segid "BrD " and resid 27   and name HN  ))
  (( segid "BrD " and resid 28   and name HB1 ))
    4.400     4.400     1.100 peak 15261 weight  0.10000E+01 volume  0.27022E+02 ppm1     8.169 ppm2     3.575
ASSI (15291)
  (( segid "BrD " and resid 26   and name HN  ))
  (( segid "BrD " and resid 24   and name HN  ))
    3.500     3.100     2.000 peak 15291 weight  0.10000E+01 volume  0.10602E+03 ppm1     9.196 ppm2     8.655
ASSI (15311)
  (( segid "BrD " and resid 25   and name HN  ))
  (( segid "BrD " and resid 24   and name HE22))
    4.900     4.900     0.600 peak 15311 weight  0.10000E+01 volume  0.14311E+02 ppm1     9.133 ppm2     7.489
ASSI (15361)
  (( segid "BrD " and resid 24   and name HN  ))
  (( segid "BrD " and resid 24   and name HE21))
    4.000     4.000     1.500 peak 15361 weight  0.10000E+01 volume  0.49074E+02 ppm1     8.659 ppm2     7.616
ASSI (15381)
  (( segid "BrD " and resid 19   and name HN  ))
  (  segid "BrD " and resid 75   and name HE% )
    5.500     5.500     0.000 peak 15381 weight  0.10000E+01 volume  0.38565E-01 ppm1     9.187 ppm2     2.654
ASSI (15391)
  (( segid "BrD " and resid 19   and name HN  ))
  (( segid "BrD " and resid 63   and name HG  ))
    4.500     4.500     1.000 peak 15391 weight  0.10000E+01 volume  0.24115E+02 ppm1     9.188 ppm2     2.454
ASSI (15401)
  (( segid "BrD " and resid 18   and name HN  ))
  (( segid "BrD " and resid 21   and name HN  ))
    3.900     3.800     1.600 peak 15401 weight  0.10000E+01 volume  0.53379E+02 ppm1     9.072 ppm2     8.558
ASSI (15421)
  (( segid "BrD " and resid 17   and name HN  ))
  (( segid "BrD " and resid 16   and name HN  ))
    2.800     2.000     2.000 peak 15421 weight  0.10000E+01 volume  0.36762E+03 ppm1     8.669 ppm2     8.780
ASSI (15441)
  (( segid "BrD " and resid 17   and name HN  ))
  (( segid "BrD " and resid 20   and name HN  ))
    3.500     3.100     2.000 peak 15441 weight  0.10000E+01 volume  0.95966E+02 ppm1     8.668 ppm2     8.184
ASSI (15481)
  (( segid "BrD " and resid 15   and name HN  ))
  (  segid "BrD " and resid 18   and name HD1%)
    5.500     5.500     0.000 peak 15481 weight  0.10000E+01 volume  0.62753E+01 ppm1     8.599 ppm2     1.069
ASSI (15511)
  (( segid "BrD " and resid 12   and name HN  ))
  (( segid "BrD " and resid 10   and name HA  ))
    3.900     3.800     1.600 peak 15511 weight  0.10000E+01 volume  0.54637E+02 ppm1     9.023 ppm2     8.464
ASSI (15531)
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   (( segid "BrD " and resid 10   and name HN  ))
   (( segid "BrD " and resid 8    and name HD2 ))
     5.200      5.200      0.300 peak 15531 weight  0.10000E+01 volume  0.99597E+01 ppm1      8.885 ppm2      4.288
ASSI {15551}
   (( segid "BrD " and resid 7    and name HN  ))
   (( segid "BrD " and resid 8    and name HD2 ))
     4.900      4.900      0.600 peak 15551 weight  0.10000E+01 volume  0.14339E+02 ppm1      8.924 ppm2      4.281
ASSI {15631}
   (( segid "BrD " and resid 32   and name HE1 ))
   (( segid "BrD " and resid 33   and name HD2 ))
     3.800      3.600      1.700 peak 15631 weight  0.10000E+01 volume  0.61547E+02 ppm1     11.082 ppm2      2.167
ASSI {15641}
   (( segid "BrD " and resid 67   and name HN  ))
   (( segid "BrD " and resid 62   and name HA  ))
     4.600      4.600      0.900 peak 15641 weight  0.10000E+01 volume  0.20420E+02 ppm1      8.832 ppm2      4.471
ASSI {27052}
   (( segid "BrD " and resid 89   and name HB1 ))
   (( segid "BrD " and resid 91   and name HD1 ))
     3.600      3.200      1.900 peak 27052 weight  0.11000E+01 volume  0.39165E+02 ppm1      3.669 ppm2      4.556
ASSI {27062}
   (( segid "BrD " and resid 89   and name HB2 ))
   (( segid "BrD " and resid 91   and name HD1 ))
     3.700      3.400      1.800 peak 27062 weight  0.11000E+01 volume  0.32055E+02 ppm1      3.473 ppm2      4.556
ASSI {27072}
   (( segid "BrD " and resid 89   and name HB2 ))
   (( segid "BrD " and resid 91   and name HD2 ))
     3.400      2.900      2.100 peak 27072 weight  0.11000E+01 volume  0.54263E+02 ppm1      3.473 ppm2      4.411
ASSI {26992}
   (( segid "BrD " and resid 89   and name HA  ))
   (( segid "BrD " and resid 91   and name HG1 ))
     3.400      2.900      2.100 peak 26992 weight  0.11000E+01 volume  0.54091E+02 ppm1      5.442 ppm2      2.792
OR {26992}
   (( segid "BrD " and resid 89   and name HA  ))
   (( segid "BrD " and resid 91   and name HG2 ))
ASSI {26732}
   (( segid "BrD " and resid 94   and name HG1 ))
   ( segid "BrD " and resid 95   and name HD% )
     3.300      2.700      2.200 peak 26732 weight  0.11000E+01 volume  0.57563E+02 ppm1      3.127 ppm2      7.505
OR {26732}
   (( segid "BrD " and resid 94   and name HG2 ))
   ( segid "BrD " and resid 95   and name HD% )
ASSI {26822}
   (( segid "BrD " and resid 94   and name HB2 ))
   ( segid "BrD " and resid 95   and name HD% )
     3.000      2.200      2.200 peak 26822 weight  0.11000E+01 volume  0.10961E+03 ppm1      2.733 ppm2      7.506
OR {26822}
   (( segid "BrD " and resid 94   and name HB1 ))
   ( segid "BrD " and resid 95   and name HD% )
ASSI {19122}
   ( segid "BrD " and resid 43   and name HB% )
   ( segid "BrD " and resid 47   and name HE% )
     3.900      3.800      1.600 peak 19122 weight  0.11000E+01 volume  0.23047E+02 ppm1      1.697 ppm2      7.267
ASSI {    2}
   (( segid "BrD " and resid 93   and name HA  ))
   (( segid "BrD " and resid 93   and name HB2 ))
     2.100      1.100      1.100 peak     2 weight  0.11000E+01 volume  0.10291E+04 ppm1      5.003 ppm2      4.766
ASSI {   22}
   (( segid "BrD " and resid 106  and name HB1 ))
   (( segid "BrD " and resid 108  and name HA  ))
     1.800      0.800      0.800 peak    22 weight  0.11000E+01 volume  0.21120E+04 ppm1      4.603 ppm2      4.801
ASSI {   32}
   (( segid "BrD " and resid 70   and name HA  ))
   (( segid "BrD " and resid 70   and name HB1 ))
     2.500      1.600      1.600 peak    32 weight  0.11000E+01 volume  0.29221E+03 ppm1      5.344 ppm2      4.786
ASSI {   62}
   (( segid "BrD " and resid 70   and name HB2 ))
   (( segid "BrD " and resid 70   and name HA  ))
     2.500      1.600      1.600 peak    62 weight  0.11000E+01 volume  0.30042E+03 ppm1      4.360 ppm2      5.360
ASSI {   72}
   (( segid "BrD " and resid 20   and name HA  ))
   (( segid "BrD " and resid 20   and name HB1 ))
     2.100      1.100      1.100 peak    72 weight  0.11000E+01 volume  0.10650E+04 ppm1      4.901 ppm2      4.670
ASSI {   92}
   (( segid "BrD " and resid 27   and name HA  ))
   (( segid "BrD " and resid 27   and name HB1 ))
     2.100      1.100      1.100 peak    92 weight  0.11000E+01 volume  0.83585E+03 ppm1      5.050 ppm2      4.617
ASSI {  112}
   (( segid "BrD " and resid 38   and name HA  ))
   ( segid "BrD " and resid 38   and name HG2% )
     2.600      1.700      1.700 peak   112 weight  0.11000E+01 volume  0.24356E+03 ppm1      4.162 ppm2      0.792
ASSI {  132}
   (( segid "BrD " and resid 38   and name HB  ))
   ( segid "BrD " and resid 38   and name HG1% )
     2.400      1.400      1.400 peak   132 weight  0.11000E+01 volume  0.41156E+03 ppm1      1.751 ppm2      1.076
ASSI {  152}
   ( segid "BrD " and resid 38   and name HG2% )
   (( segid "BrD " and resid 38   and name HB  ))
     2.300      1.300      1.300 peak   152 weight  0.11000E+01 volume  0.59973E+03 ppm1      0.808 ppm2      1.776
ASSI {  232}
   (( segid "BrD " and resid 81   and name HB  ))
   ( segid "BrD " and resid 81   and name HG1% )
     2.400      1.400      1.400 peak   232 weight  0.11000E+01 volume  0.37086E+03 ppm1      2.042 ppm2      1.079
ASSI {  242}
   (( segid "BrD " and resid 81   and name HB  ))
   ( segid "BrD " and resid 81   and name HG2% )
     2.300      1.300      1.300 peak   242 weight  0.11000E+01 volume  0.47548E+03 ppm1      2.042 ppm2      0.759
ASSI {  262}
   (( segid "BrD " and resid 15   and name HA  ))
   (( segid "BrD " and resid 15   and name HB1 ))
     2.700      1.800      1.800 peak   262 weight  0.11000E+01 volume  0.20830E+03 ppm1      4.607 ppm2      3.811
ASSI {  322}
   (( segid "BrD " and resid 46   and name HB1 ))
   (( segid "BrD " and resid 46   and name HA  ))
     2.700      1.800      1.800 peak   322 weight  0.11000E+01 volume  0.21305E+03 ppm1      3.274 ppm2      4.143
ASSI {  332}
   (( segid "BrD " and resid 46   and name HB2 ))
   (( segid "BrD " and resid 46   and name HA  ))
     2.700      1.800      1.800 peak   332 weight  0.11000E+01 volume  0.21514E+03 ppm1      3.077 ppm2      4.143
ASSI {  352}
   (( segid "BrD " and resid 47   and name HA  ))
   (( segid "BrD " and resid 47   and name HB2 ))
     2.700      1.800      1.800 peak   352 weight  0.11000E+01 volume  0.22249E+03 ppm1      4.704 ppm2      3.395
ASSI {  362}
   (( segid "BrD " and resid 47   and name HB1 ))
   (( segid "BrD " and resid 47   and name HA  ))
     2.600      1.700      1.700 peak   362 weight  0.11000E+01 volume  0.23254E+03 ppm1      3.815 ppm2      4.721
ASSI {  382}
   (( segid "BrD " and resid 67   and name HA  ))
   (( segid "BrD " and resid 67   and name HB1 ))
     2.400      1.400      1.400 peak   382 weight  0.11000E+01 volume  0.45818E+03 ppm1      4.654 ppm2      3.572
ASSI {  392}
   (( segid "BrD " and resid 67   and name HA  ))
   (( segid "BrD " and resid 67   and name HB2 ))
     2.500      1.600      1.600 peak   392 weight  0.11000E+01 volume  0.31584E+03 ppm1      4.653 ppm2      2.669
ASSI {  422}
   (( segid "BrD " and resid 68   and name HB1 ))
   (( segid "BrD " and resid 68   and name HA  ))
     3.100      2.400      2.400 peak   422 weight  0.11000E+01 volume  0.94493E+02 ppm1      3.668 ppm2      5.143
ASSI {  432}
   (( segid "BrD " and resid 68   and name HB2 ))
   (( segid "BrD " and resid 68   and name HA  ))
     2.700      1.800      1.800 peak   432 weight  0.11000E+01 volume  0.18471E+03 ppm1      3.522 ppm2      5.143
ASSI {  472}
   (( segid "BrD " and resid 88   and name HB1 ))
   (( segid "BrD " and resid 88   and name HA  ))
     2.600      1.700      1.700 peak   472 weight  0.11000E+01 volume  0.26741E+03 ppm1      3.522 ppm2      4.989
ASSI {  492}
   (( segid "BrD " and resid 95   and name HA  ))
   (( segid "BrD " and resid 95   and name HB2 ))
     2.600      1.700      1.700 peak   492 weight  0.11000E+01 volume  0.23932E+03 ppm1      4.459 ppm2      3.361
ASSI {  502}
   (( segid "BrD " and resid 95   and name HB1 ))
   (( segid "BrD " and resid 95   and name HA  ))
     2.600      1.700      1.700 peak   502 weight  0.11000E+01 volume  0.28555E+03 ppm1      3.619 ppm2      4.444
ASSI {  522}
   (( segid "BrD " and resid 96   and name HA  ))
   (( segid "BrD " and resid 96   and name HB1 ))
     2.800      2.000      2.000 peak   522 weight  0.11000E+01 volume  0.17185E+03 ppm1      4.409 ppm2      3.998
ASSI {  532}
   (( segid "BrD " and resid 96   and name HA  ))
   (( segid "BrD " and resid 96   and name HB2 ))
     2.800      2.000      2.000 peak   532 weight  0.11000E+01 volume  0.16898E+03 ppm1      4.409 ppm2      3.118
ASSI {  562}
   (( segid "BrD " and resid 31   and name HA  ))
   ( segid "BrD " and resid 31   and name HB% )
     2.500      1.600      1.600 peak   562 weight  0.11000E+01 volume  0.36356E+03 ppm1      5.000 ppm2      2.318
ASSI {  592}
   ( segid "BrD " and resid 43   and name HB% )
   (( segid "BrD " and resid 43   and name HA  ))
     2.200      1.200      1.200 peak   592 weight  0.11000E+01 volume  0.76123E+03 ppm1      1.700 ppm2      5.539
ASSI {  612}
   ( segid "BrD " and resid 76   and name HB% )
   (( segid "BrD " and resid 76   and name HA  ))
     2.100      1.100      1.100 peak   612 weight  0.11000E+01 volume  0.87848E+03 ppm1      2.093 ppm2      4.687
ASSI {  632}
   ( segid "BrD " and resid 99   and name HB% )
   (( segid "BrD " and resid 99   and name HA  ))
     2.000      1.000      1.000 peak   632 weight  0.11000E+01 volume  0.10742E+04 ppm1      2.190 ppm2      4.440
ASSI {  642}
   (( segid "BrD " and resid 113  and name HA  ))
   ( segid "BrD " and resid 113  and name HB% )
     2.100      1.100      1.100 peak   642 weight  0.11000E+01 volume  0.84264E+03 ppm1      4.901 ppm2      1.979
ASSI {  662}
   (( segid "BrD " and resid 34   and name HA  ))
   (( segid "BrD " and resid 34   and name HB1 ))
     2.600      1.700      1.700 peak   662 weight  0.11000E+01 volume  0.27701E+03 ppm1      5.542 ppm2      4.107
ASSI {  672}
   (( segid "BrD " and resid 34   and name HA  ))
   (( segid "BrD " and resid 34   and name HB2 ))
     2.800      2.000      2.000 peak   672 weight  0.11000E+01 volume  0.16922E+03 ppm1      5.542 ppm2      3.146
ASSI {  702}
   (( segid "BrD " and resid 74   and name HA  ))
   (( segid "BrD " and resid 74   and name HB1 ))
     3.000      2.200      2.200 peak   702 weight  0.11000E+01 volume  0.10996E+03 ppm1      4.359 ppm2      3.563
ASSI {  712}
   (( segid "BrD " and resid 74   and name HA  ))
   (( segid "BrD " and resid 74   and name HB2 ))
     3.100      2.400      2.400 peak   712 weight  0.11000E+01 volume  0.88126E+02 ppm1      4.361 ppm2      3.000
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ASSI ( 742)
   (( segid "BrD " and resid 82   and name HA  ))
   (( segid "BrD " and resid 82   and name HB1 ))
     2.800     2.000     2.000 peak   742 weight  0.11000E+01 volume  0.15835E+03 ppm1      4.755 ppm2      3.695
ASSI ( 752)
   (( segid "BrD " and resid 82   and name HA  ))
   (( segid "BrD " and resid 82   and name HB2 ))
     2.700     1.800     1.800 peak   752 weight  0.11000E+01 volume  0.16532E+03 ppm1      4.755 ppm2      3.573
ASSI ( 792)
   (( segid "BrD " and resid 106  and name HA  ))
   (( segid "BrD " and resid 106  and name HB1 ))
     2.700     1.800     1.800 peak   792 weight  0.11000E+01 volume  0.19130E+03 ppm1      4.558 ppm2      3.916
ASSI ( 802)
   (( segid "BrD " and resid 106  and name HA  ))
   (( segid "BrD " and resid 106  and name HB2 ))
     2.600     1.700     1.700 peak   802 weight  0.11000E+01 volume  0.25966E+03 ppm1      4.557 ppm2      3.702
ASSI ( 842)
   (( segid "BrD " and resid 107  and name HB1 ))
   (( segid "BrD " and resid 107  and name HA  ))
     2.200     1.200     1.200 peak   842 weight  0.11000E+01 volume  0.64742E+03 ppm1      3.671 ppm2      4.435
ASSI ( 872)
   (( segid "BrD " and resid 65   and name HA  ))
   (( segid "BrD " and resid 65   and name HB1 ))
     2.600     1.700     1.700 peak   872 weight  0.11000E+01 volume  0.23368E+03 ppm1      5.398 ppm2      3.621
ASSI ( 882)
   (( segid "BrD " and resid 65   and name HA  ))
   (( segid "BrD " and resid 65   and name HB2 ))
     2.900     2.100     2.100 peak   882 weight  0.11000E+01 volume  0.14380E+03 ppm1      5.396 ppm2      3.369
ASSI ( 892)
   (( segid "BrD " and resid 84   and name HA  ))
   (( segid "BrD " and resid 84   and name HB1 ))
     2.700     1.800     1.800 peak   892 weight  0.11000E+01 volume  0.20950E+03 ppm1      4.904 ppm2      3.606
ASSI ( 902)
   (( segid "BrD " and resid 84   and name HA  ))
   (( segid "BrD " and resid 84   and name HB2 ))
     2.600     1.700     1.700 peak   902 weight  0.11000E+01 volume  0.23639E+03 ppm1      4.904 ppm2      3.272
ASSI ( 942)
   (( segid "BrD " and resid 100  and name HB2 ))
   (( segid "BrD " and resid 100  and name HA  ))
     2.300     1.300     1.300 peak   942 weight  0.11000E+01 volume  0.53744E+03 ppm1      3.424 ppm2      4.949
ASSI ( 952)
   (( segid "BrD " and resid 10   and name HA  ))
   (( segid "BrD " and resid 10   and name HB1 ))
     3.200     2.600     2.300 peak   952 weight  0.11000E+01 volume  0.81254E+02 ppm1      5.478 ppm2      3.354
ASSI ( 972)
   (( segid "BrD " and resid 12   and name HA  ))
   (( segid "BrD " and resid 12   and name HB1 ))
     2.700     1.800     1.800 peak   972 weight  0.11000E+01 volume  0.22766E+03 ppm1      5.297 ppm2      3.434
ASSI ( 992)
   (( segid "BrD " and resid 77   and name HA  ))
   (( segid "BrD " and resid 77   and name HB1 ))
     2.500     1.600     1.600 peak   992 weight  0.11000E+01 volume  0.33274E+03 ppm1      4.951 ppm2      3.319
ASSI ( 1032)
   (( segid "BrD " and resid 117  and name HB2 ))
   (( segid "BrD " and resid 117  and name HA  ))
     2.700     1.800     1.800 peak  1032 weight  0.11000E+01 volume  0.21830E+03 ppm1      3.127 ppm2      5.167
ASSI ( 1042)
   (( segid "BrD " and resid 117  and name HB1 ))
   (( segid "BrD " and resid 117  and name HA  ))
     2.600     1.700     1.700 peak  1042 weight  0.11000E+01 volume  0.23430E+03 ppm1      3.301 ppm2      5.167
ASSI ( 1052)
   (( segid "BrD " and resid 89   and name HA  ))
   (( segid "BrD " and resid 89   and name HB1 ))
     2.900     2.100     2.100 peak  1052 weight  0.11000E+01 volume  0.12958E+03 ppm1      5.641 ppm2      3.668
ASSI ( 1062)
   (( segid "BrD " and resid 89   and name HA  ))
   (( segid "BrD " and resid 89   and name HB2 ))
     2.800     2.000     2.000 peak  1062 weight  0.11000E+01 volume  0.16727E+03 ppm1      5.641 ppm2      3.491
ASSI ( 1092)
   (( segid "BrD " and resid 18   and name HA  ))
   (( segid "BrD " and resid 18   and name HG  ))
     3.100     2.400     2.400 peak  1092 weight  0.11000E+01 volume  0.85824E+02 ppm1      3.866 ppm2      2.277
ASSI ( 1132)
   (  segid "BrD " and resid 18   and name HD2%)
   (( segid "BrD " and resid 18   and name HA  ))
     2.100     1.100     1.100 peak  1132 weight  0.11000E+01 volume  0.86347E+03 ppm1      0.415 ppm2      3.883
ASSI ( 1142)
   (  segid "BrD " and resid 18   and name HD2%)
   (( segid "BrD " and resid 18   and name HG  ))
     2.500     1.600     1.600 peak  1142 weight  0.11000E+01 volume  0.31482E+03 ppm1      0.419 ppm2      2.274
ASSI ( 1162)
   (( segid "BrD " and resid 78   and name HA  ))
   (( segid "BrD " and resid 78   and name HB2 ))
     2.500     1.600     1.600 peak  1162 weight  0.11000E+01 volume  0.33654E+03 ppm1      3.968 ppm2      1.044
ASSI ( 1172)
   (( segid "BrD " and resid 78   and name HA  ))
   (( segid "BrD " and resid 78   and name HG  ))
     2.900     2.100     2.100 peak  1172 weight  0.11000E+01 volume  0.14454E+03 ppm1      3.967 ppm2      1.270
ASSI ( 1202)
   (( segid "BrD " and resid 78   and name HB1 ))
   (( segid "BrD " and resid 78   and name HA  ))
     2.700     1.800     1.800 peak  1202 weight  0.11000E+01 volume  0.21643E+03 ppm1      1.305 ppm2      4.001
ASSI ( 1212)
   (( segid "BrD " and resid 78   and name HB1 ))
   (  segid "BrD " and resid 78   and name HD1%)
     2.900     2.100     2.100 peak  1212 weight  0.11000E+01 volume  0.13310E+03 ppm1      1.305 ppm2      0.776
ASSI ( 1222)
   (( segid "BrD " and resid 78   and name HB1 ))
   (  segid "BrD " and resid 78   and name HD2%)
     2.700     1.800     1.800 peak  1222 weight  0.11000E+01 volume  0.22009E+03 ppm1      1.305 ppm2      0.673
ASSI ( 1262)
   (( segid "BrD " and resid 78   and name HG  ))
   (( segid "BrD " and resid 78   and name HB2 ))
     2.400     1.400     1.400 peak  1262 weight  0.11000E+01 volume  0.41554E+03 ppm1      1.254 ppm2      1.043
ASSI ( 1282)
   (  segid "BrD " and resid 78   and name HD1%)
   (( segid "BrD " and resid 78   and name HA  ))
     2.400     1.400     1.400 peak  1282 weight  0.11000E+01 volume  0.38399E+03 ppm1      0.761 ppm2      3.998
ASSI ( 1302)
   (  segid "BrD " and resid 78   and name HD1%)
   (( segid "BrD " and resid 78   and name HB2 ))
     2.600     1.700     1.700 peak  1302 weight  0.11000E+01 volume  0.25846E+03 ppm1      0.761 ppm2      1.038
ASSI ( 1312)
   (  segid "BrD " and resid 78   and name HD1%)
   (( segid "BrD " and resid 78   and name HG  ))
     2.200     1.200     1.200 peak  1312 weight  0.11000E+01 volume  0.70030E+03 ppm1      0.761 ppm2      1.270
ASSI ( 1322)
   (( segid "BrD " and resid 115  and name HA  ))
   (( segid "BrD " and resid 115  and name HB1 ))
     2.200     1.200     1.200 peak  1322 weight  0.11000E+01 volume  0.70481E+03 ppm1      4.807 ppm2      2.182
ASSI ( 1352)
   (  segid "BrD " and resid 115  and name HD1%)
   (( segid "BrD " and resid 115  and name HA  ))
     1.100     2.700     2.200 peak  1352 weight  0.11000E+01 volume  0.57522E+02 ppm1      1.352 ppm2      4.839
ASSI ( 1362)
   (  segid "BrD " and resid 115  and name HD1%)
   (( segid "BrD " and resid 115  and name HG  ))
     2.400     1.400     1.400 peak  1362 weight  0.11000E+01 volume  0.44618E+03 ppm1      1.352 ppm2      2.148
ASSI ( 1382)
   (( segid "BrD " and resid 116  and name HB  ))
   (( segid "BrD " and resid 116  and name HA  ))
     2.700     1.800     1.800 peak  1382 weight  0.11000E+01 volume  0.19754E+03 ppm1      2.411 ppm2      4.823
ASSI ( 1402)
   (( segid "BrD " and resid 116  and name HB  ))
   (( segid "BrD " and resid 116  and name HG12))
     2.200     1.200     1.200 peak  1402 weight  0.11000E+01 volume  0.69385E+03 ppm1      2.409 ppm2      1.555
ASSI ( 1422)
   (( segid "BrD " and resid 116  and name HG11))
   (( segid "BrD " and resid 116  and name HB  ))
     2.500     1.600     1.600 peak  1422 weight  0.11000E+01 volume  0.30727E+03 ppm1      1.920 ppm2      2.418
ASSI ( 1432)
   (  segid "BrD " and resid 116  and name HG2%)
   (( segid "BrD " and resid 116  and name HA  ))
     2.500     1.600     1.600 peak  1432 weight  0.11000E+01 volume  0.32118E+03 ppm1      1.403 ppm2      4.823
ASSI ( 1442)
   (  segid "BrD " and resid 116  and name HG2%)
   (( segid "BrD " and resid 116  and name HB  ))
     2.300     1.300     1.300 peak  1442 weight  0.11000E+01 volume  0.50062E+03 ppm1      1.403 ppm2      2.419
ASSI ( 1452)
   (  segid "BrD " and resid 116  and name HD1%)
   (( segid "BrD " and resid 116  and name HG12))
     2.100     1.100     1.100 peak  1452 weight  0.11000E+01 volume  0.85569E+03 ppm1      1.399 ppm2      1.554
ASSI ( 1462)
   (  segid "BrD " and resid 116  and name HD1%)
   (( segid "BrD " and resid 116  and name HG11))
     2.500     1.600     1.600 peak  1462 weight  0.11000E+01 volume  0.33669E+03 ppm1      1.399 ppm2      1.919
ASSI ( 1512)
   (( segid "BrD " and resid 110  and name HB  ))
   (( segid "BrD " and resid 110  and name HA  ))
     2.400     1.400     1.400 peak  1512 weight  0.11000E+01 volume  0.40202E+03 ppm1      2.338 ppm2      4.418
ASSI ( 1542)
   (  segid "BrD " and resid 110  and name HG2%)
   (( segid "BrD " and resid 110  and name HA  ))
     2.200     1.200     1.200 peak  1542 weight  0.11000E+01 volume  0.74299E+03 ppm1      1.251 ppm2      4.418
ASSI ( 1552)
   (  segid "BrD " and resid 110  and name HG2%)
   (( segid "BrD " and resid 110  and name HB  ))
     2.200     1.200     1.200 peak  1552 weight  0.11000E+01 volume  0.70453E+03 ppm1      1.252 ppm2      2.361
ASSI ( 1562)
   (  segid "BrD " and resid 110  and name HG2%)
   (( segid "BrD " and resid 110  and name HG11))
     2.600     1.700     1.700 peak  1562 weight  0.11000E+01 volume  0.27736E+03 ppm1      1.253 ppm2      1.718
ASSI ( 1572)
   (  segid "BrD " and resid 110  and name HG2%)
   (  segid "BrD " and resid 110  and name HD1%)
     2.000     1.000     1.000 peak  1572 weight  0.11000E+01 volume  0.13448E+04 ppm1      1.254 ppm2      1.141
ASSI ( 1602)
   (  segid "BrD " and resid 110  and name HD1%)
   (( segid "BrD " and resid 110  and name HA  ))
     2.200     1.200     1.200 peak  1602 weight  0.11000E+01 volume  0.74125E+03 ppm1      1.154 ppm2      4.420
ASSI ( 1612)
   (  segid "BrD " and resid 110  and name HD1%)
   (( segid "BrD " and resid 110  and name HB  ))
     2.200     1.200     1.200 peak  1612 weight  0.11000E+01 volume  0.75209E+03 ppm1      1.154 ppm2      2.361
ASSI ( 1622)
   (  segid "BrD " and resid 110  and name HD1%)
   (( segid "BrD " and resid 110  and name HG11))
     2.300     1.300     1.300 peak  1622 weight  0.11000E+01 volume  0.59823E+03 ppm1      1.154 ppm2      1.718
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ASSI { 1682}
  ( segid "BrD " and resid 50   and name HD1%)
  (( segid "BrD " and resid 50   and name HB  ))
    2.800     2.000     2.000 peak  1682 weight  0.11000E+01 volume  0.14989E+03 ppm1      1.154 ppm2      1.826
ASSI { 1692}
  ( segid "BrD " and resid 50   and name HD1%)
  (( segid "BrD " and resid 50   and name HG11))
    2.300     1.300     1.300 peak  1692 weight  0.11000E+01 volume  0.49711E+03 ppm1      1.154 ppm2      1.408
ASSI { 1702}
  ( segid "BrD " and resid 50   and name HD1%)
  (( segid "BrD " and resid 50   and name HG12))
    2.400     1.400     1.400 peak  1702 weight  0.11000E+01 volume  0.46662E+03 ppm1      1.155 ppm2      0.838
ASSI { 1712}
  ( segid "BrD " and resid 50   and name HD1%)
  ( segid "BrD " and resid 50   and name HG2%)
    2.400     1.400     1.400 peak  1712 weight  0.11000E+01 volume  0.45288E+03 ppm1      1.154 ppm2      0.994
ASSI { 1742}
  ( segid "BrD " and resid 50   and name HG2%)
  (( segid "BrD " and resid 50   and name HA  ))
    2.400     1.400     1.400 peak  1742 weight  0.11000E+01 volume  0.43004E+03 ppm1      1.006 ppm2      4.518
ASSI { 1752}
  ( segid "BrD " and resid 50   and name HG2%)
  (( segid "BrD " and resid 50   and name HB  ))
    2.200     1.200     1.200 peak  1752 weight  0.11000E+01 volume  0.61665E+03 ppm1      1.006 ppm2      1.825
ASSI { 1762}
  ( segid "BrD " and resid 50   and name HG2%)
  (( segid "BrD " and resid 50   and name HG11))
    2.800     2.000     2.000 peak  1762 weight  0.11000E+01 volume  0.16808E+03 ppm1      1.008 ppm2      1.409
ASSI { 1772}
  ( segid "BrD " and resid 50   and name HG2%)
  (( segid "BrD " and resid 50   and name HG12))
    2.400     1.400     1.400 peak  1772 weight  0.11000E+01 volume  0.40990E+03 ppm1      1.006 ppm2      0.838
ASSI { 1792}
  (( segid "BrD " and resid 101  and name HA  ))
  ( segid "BrD " and resid 101  and name HD1%)
    2.700     1.800     1.800 peak  1792 weight  0.11000E+01 volume  0.20691E+03 ppm1      4.261 ppm2      1.578
ASSI { 1812}
  (( segid "BrD " and resid 101  and name HB  ))
  ( segid "BrD " and resid 101  and name HD1%)
    2.300     1.300     1.300 peak  1812 weight  0.11000E+01 volume  0.50350E+03 ppm1      2.537 ppm2      1.578
ASSI { 1852}
  (( segid "BrD " and resid 101  and name HG11))
  ( segid "BrD " and resid 101  and name HG2%)
    2.600     1.700     1.700 peak  1852 weight  0.11000E+01 volume  0.23958E+03 ppm1      2.444 ppm2      1.609
ASSI { 1872}
  ( segid "BrD " and resid 101  and name HG2%)
  (( segid "BrD " and resid 101  and name HA  ))
    2.400     1.400     1.400 peak  1872 weight  0.11000E+01 volume  0.44349E+03 ppm1      1.596 ppm2      4.265
ASSI { 1882}
  ( segid "BrD " and resid 101  and name HG2%)
  (( segid "BrD " and resid 101  and name HB  ))
    2.200     1.200     1.200 peak  1882 weight  0.11000E+01 volume  0.72150E+03 ppm1      1.600 ppm2      2.536
ASSI { 1892}
  ( segid "BrD " and resid 101  and name HG2%)
  (( segid "BrD " and resid 101  and name HG12))
    2.300     1.300     1.300 peak  1892 weight  0.11000E+01 volume  0.60307E+03 ppm1      1.598 ppm2      1.806
ASSI { 1922}
  ( segid "BrD " and resid 101  and name HD1%)
  (( segid "BrD " and resid 101  and name HG11))
    2.300     1.300     1.300 peak  1922 weight  0.11000E+01 volume  0.50142E+03 ppm1      1.550 ppm2      2.467
ASSI { 1932}
  ( segid "BrD " and resid 101  and name HD1%)
  (( segid "BrD " and resid 101  and name HG12))
    2.200     1.200     1.200 peak  1932 weight  0.11000E+01 volume  0.71179E+03 ppm1      1.550 ppm2      1.806
ASSI { 1952}
  (( segid "BrD " and resid 21   and name HA  ))
  ( segid "BrD " and resid 21   and name HD1%)
    2.800     2.000     2.000 peak  1952 weight  0.11000E+01 volume  0.16491E+03 ppm1      4.359 ppm2      1.221
ASSI { 1962}
  (( segid "BrD " and resid 21   and name HB  ))
  ( segid "BrD " and resid 21   and name HG2%)
    3.100     2.400     2.400 peak  1962 weight  0.11000E+01 volume  0.84008E+02 ppm1      2.487 ppm2      1.588
ASSI { 1982}
  (( segid "BrD " and resid 21   and name HG12))
  ( segid "BrD " and resid 21   and name HD1%)
    2.500     1.600     1.600 peak  1982 weight  0.11000E+01 volume  0.32678E+03 ppm1      1.648 ppm2      1.222
ASSI { 2012}
  ( segid "BrD " and resid 21   and name HG2%)
  (( segid "BrD " and resid 21   and name HG11))
    2.600     1.700     1.700 peak  2012 weight  0.11000E+01 volume  0.24142E+03 ppm1      1.598 ppm2      2.357
ASSI { 2022}
  ( segid "BrD " and resid 21   and name HD1%)
  (( segid "BrD " and resid 21   and name HB  ))
    2.500     1.600     1.600 peak  2022 weight  0.11000E+01 volume  0.29587E+03 ppm1      1.206 ppm2      2.508
ASSI { 2032}
  ( segid "BrD " and resid 21   and name HD1%)
  (( segid "BrD " and resid 21   and name HG11))
    2.400     1.400     1.400 peak  2032 weight  0.11000E+01 volume  0.44094E+03 ppm1      1.205 ppm2      2.355
ASSI { 2042}
  ( segid "BrD " and resid 21   and name HD1%)
  ( segid "BrD " and resid 21   and name HG2%)
    2.300     1.300     1.300 peak  2042 weight  0.11000E+01 volume  0.49870E+03 ppm1      1.208 ppm2      1.584
ASSI { 2052}
  (( segid "BrD " and resid 112  and name HA  ))
  (( segid "BrD " and resid 112  and name HG1 ))
    2.700     1.800     1.800 peak  2052 weight  0.11000E+01 volume  0.21076E+03 ppm1      4.607 ppm2      2.942
ASSI { 2072}
  (( segid "BrD " and resid 112  and name HB1 ))
  (( segid "BrD " and resid 112  and name HG1 ))
    2.300     1.300     1.300 peak  2072 weight  0.11000E+01 volume  0.51152E+03 ppm1      2.684 ppm2      2.947
ASSI { 2092}
  (( segid "BrD " and resid 94   and name HA  ))
  (( segid "BrD " and resid 94   and name HG1 ))
    2.700     1.800     1.800 peak  2092 weight  0.11000E+01 volume  0.21281E+03 ppm1      4.830 ppm2      3.127
ASSI { 2112}
  (( segid "BrD " and resid 92   and name HG1 ))
  (( segid "BrD " and resid 92   and name HA  ))
    2.400     1.400     1.400 peak  2112 weight  0.11000E+01 volume  0.46860E+03 ppm1      2.816 ppm2      4.798
ASSI { 2142}
  (( segid "BrD " and resid 87   and name HG1 ))
  (( segid "BrD " and resid 87   and name HA  ))
    2.900     2.100     2.100 peak  2142 weight  0.11000E+01 volume  0.13435E+03 ppm1      3.030 ppm2      4.874
ASSI { 2152}
  (( segid "BrD " and resid 87   and name HG2 ))
  (( segid "BrD " and resid 87   and name HA  ))
    2.500     1.600     1.600 peak  2152 weight  0.11000E+01 volume  0.35437E+03 ppm1      2.782 ppm2      4.875
ASSI { 2172}
  (( segid "BrD " and resid 61   and name HG1 ))
  (( segid "BrD " and resid 61   and name HA  ))
    2.300     1.300     1.300 peak  2172 weight  0.11000E+01 volume  0.47499E+03 ppm1      2.980 ppm2      4.670
ASSI { 2182}
  (( segid "BrD " and resid 61   and name HG2 ))
  (( segid "BrD " and resid 61   and name HA  ))
    2.800     2.000     2.000 peak  2182 weight  0.11000E+01 volume  0.17452E+03 ppm1      2.832 ppm2      4.670
ASSI { 2202}
  (( segid "BrD " and resid 42   and name HG1 ))
  (( segid "BrD " and resid 42   and name HA  ))
    2.400     1.400     1.400 peak  2202 weight  0.11000E+01 volume  0.43794E+03 ppm1      2.880 ppm2      5.049
ASSI { 2222}
  (( segid "BrD " and resid 36   and name HG1 ))
  (( segid "BrD " and resid 36   and name HA  ))
    2.600     1.700     1.700 peak  2222 weight  0.11000E+01 volume  0.28226E+03 ppm1      2.781 ppm2      5.445
ASSI { 2252}
  (( segid "BrD " and resid 79   and name HG1 ))
  (( segid "BrD " and resid 79   and name HA  ))
    2.600     1.700     1.700 peak  2252 weight  0.11000E+01 volume  0.27675E+03 ppm1      3.033 ppm2      4.417
ASSI { 2262}
  (( segid "BrD " and resid 29   and name HA  ))
  (( segid "BrD " and resid 29   and name HB1 ))
    2.000     1.000     1.000 peak  2262 weight  0.11000E+01 volume  0.11521E+04 ppm1      4.810 ppm2      2.738
ASSI { 2272}
  (( segid "BrD " and resid 29   and name HG1 ))
  (( segid "BrD " and resid 29   and name HA  ))
    2.600     1.700     1.700 peak  2272 weight  0.11000E+01 volume  0.24467E+03 ppm1      2.980 ppm2      4.810
ASSI { 2302}
  (( segid "BrD " and resid 23   and name HG1 ))
  (( segid "BrD " and resid 23   and name HA  ))
    2.500     1.600     1.600 peak  2302 weight  0.11000E+01 volume  0.32948E+03 ppm1      3.124 ppm2      4.638
ASSI { 2312}
  (( segid "BrD " and resid 23   and name HG2 ))
  (( segid "BrD " and resid 23   and name HA  ))
    2.400     1.400     1.400 peak  2312 weight  0.11000E+01 volume  0.37520E+03 ppm1      3.068 ppm2      4.638
ASSI { 2322}
  (( segid "BrD " and resid 80   and name HG2 ))
  (( segid "BrD " and resid 80   and name HG1 ))
    2.500     1.600     1.600 peak  2322 weight  0.11000E+01 volume  0.34874E+03 ppm1      3.913 ppm2      2.367
ASSI { 2342}
  (( segid "BrD " and resid 80   and name HD2 ))
  (( segid "BrD " and resid 80   and name HB1 ))
    2.800     2.000     2.000 peak  2342 weight  0.11000E+01 volume  0.17327E+03 ppm1      3.913 ppm2      2.573
ASSI { 2372}
  (( segid "BrD " and resid 66   and name HA  ))
  (( segid "BrD " and resid 66   and name HD1 ))
    2.700     1.800     1.800 peak  2372 weight  0.11000E+01 volume  0.22456E+03 ppm1      5.000 ppm2      3.670
ASSI { 2382}
  (( segid "BrD " and resid 66   and name HG2 ))
  (( segid "BrD " and resid 66   and name HD1 ))
    2.500     1.600     1.600 peak  2382 weight  0.11000E+01 volume  0.35872E+03 ppm1      2.140 ppm2      3.670
ASSI { 2392}
  (( segid "BrD " and resid 9    and name HD1 ))
  (( segid "BrD " and resid 9    and name HG1 ))
    2.300     1.300     1.300 peak  2392 weight  0.11000E+01 volume  0.51278E+03 ppm1      3.769 ppm2      2.279
ASSI { 2432}
  (( segid "BrD " and resid 35   and name HG1 ))
  (( segid "BrD " and resid 35   and name HA  ))
    2.900     2.100     2.100 peak  2432 weight  0.11000E+01 volume  0.13495E+03 ppm1      3.422 ppm2      4.901
ASSI { 2442}
  (( segid "BrD " and resid 102  and name HB1 ))
  (( segid "BrD " and resid 102  and name HA  ))
    2.700     1.800     1.800 peak  2442 weight  0.11000E+01 volume  0.22859E+03 ppm1      1.994 ppm2      4.282
ASSI { 2452}
  (( segid "BrD " and resid 102  and name HB2 ))
  (( segid "BrD " and resid 102  and name HA  ))
    2.700     1.800     1.800 peak  2452 weight  0.11000E+01 volume  0.18482E+03 ppm1      1.848 ppm2      4.280
ASSI { 2462}
  (( segid "BrD " and resid 102  and name HB1 ))
  ( segid "BrD " and resid 102  and name HD1%)
    2.500     1.600     1.600 peak  2462 weight  0.11000E+01 volume  0.28966E+03 ppm1      1.992 ppm2      1.325
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ASSI { 2472}
  (( segid "BrD " and resid 102  and name HB2 ))
  (  segid "BrD " and resid 102  and name HD1%)
     2.500     1.600     1.600 peak  2472 weight  0.11000E+01 volume  0.33733E+03 ppm1     1.842 ppm2     1.325
ASSI { 2532}
  (( segid "BrD " and resid 73   and name HA  ))
  (( segid "BrD " and resid 73   and name HB2 ))
     2.500     1.600     1.600 peak  2532 weight  0.11000E+01 volume  0.31007E+03 ppm1     4.805 ppm2     2.482
ASSI { 2542}
  (( segid "BrD " and resid 73   and name HA  ))
  (( segid "BrD " and resid 73   and name HG  ))
     2.600     1.700     1.700 peak  2542 weight  0.11000E+01 volume  0.27034E+03 ppm1     4.805 ppm2     2.368
ASSI { 2572}
  (( segid "BrD " and resid 73   and name HB2 ))
  (  segid "BrD " and resid 73   and name HD1%)
     2.400     1.400     1.400 peak  2572 weight  0.11000E+01 volume  0.37597E+03 ppm1     2.487 ppm2     1.539
ASSI { 2582}
  (  segid "BrD " and resid 73   and name HD2%)
  (( segid "BrD " and resid 73   and name HA  ))
     2.200     1.200     1.200 peak  2582 weight  0.11000E+01 volume  0.64867E+03 ppm1     1.499 ppm2     4.827
ASSI { 2592}
  (  segid "BrD " and resid 73   and name HD2%)
  (( segid "BrD " and resid 73   and name HG  ))
     2.100     1.100     1.100 peak  2592 weight  0.11000E+01 volume  0.88262E+03 ppm1     1.500 ppm2     2.367
ASSI { 2602}
  (  segid "BrD " and resid 56   and name HD2%)
  (( segid "BrD " and resid 56   and name HG  ))
     2.200     1.200     1.200 peak  2602 weight  0.11000E+01 volume  0.64971E+03 ppm1     1.254 ppm2     2.328
ASSI { 2612}
  (  segid "BrD " and resid 56   and name HD2%)
  (( segid "BrD " and resid 56   and name HB1 ))
     2.700     1.800     1.800 peak  2612 weight  0.11000E+01 volume  0.20000E+03 ppm1     1.254 ppm2     2.703
ASSI { 2622}
  (  segid "BrD " and resid 56   and name HD2%)
  (( segid "BrD " and resid 56   and name HA  ))
     2.200     1.200     1.200 peak  2622 weight  0.11000E+01 volume  0.63602E+03 ppm1     1.253 ppm2     4.630
ASSI { 2652}
  (( segid "BrD " and resid 22   and name HB1 ))
  (( segid "BrD " and resid 22   and name HA  ))
     2.400     1.400     1.400 peak  2652 weight  0.11000E+01 volume  0.44257E+03 ppm1     2.682 ppm2     4.723
ASSI { 2662}
  (( segid "BrD " and resid 22   and name HB2 ))
  (( segid "BrD " and resid 22   and name HA  ))
     2.400     1.400     1.400 peak  2662 weight  0.11000E+01 volume  0.37194E+03 ppm1     2.287 ppm2     4.723
ASSI { 2682}
  (  segid "BrD " and resid 22   and name HD2%)
  (( segid "BrD " and resid 22   and name HA  ))
     2.200     1.200     1.200 peak  2682 weight  0.11000E+01 volume  0.64884E+03 ppm1     1.599 ppm2     4.723
ASSI { 2702}
  (( segid "BrD " and resid 63   and name HA  ))
  (( segid "BrD " and resid 63   and name HB1 ))
     2.900     2.100     2.100 peak  2702 weight  0.11000E+01 volume  0.13727E+03 ppm1     5.296 ppm2     2.907
ASSI { 2712}
  (( segid "BrD " and resid 63   and name HA  ))
  (( segid "BrD " and resid 63   and name HB2 ))
     2.700     1.800     1.800 peak  2712 weight  0.11000E+01 volume  0.18645E+03 ppm1     5.296 ppm2     2.535
ASSI { 2722}
  (( segid "BrD " and resid 63   and name HA  ))
  (( segid "BrD " and resid 63   and name HG  ))
     2.900     2.100     2.100 peak  2722 weight  0.11000E+01 volume  0.13509E+03 ppm1     5.293 ppm2     2.423
ASSI { 2732}
  (( segid "BrD " and resid 63   and name HA  ))
  (  segid "BrD " and resid 63   and name HD1%)
     2.700     1.800     1.800 peak  2732 weight  0.11000E+01 volume  0.22485E+03 ppm1     5.296 ppm2     1.649
ASSI { 2742}
  (( segid "BrD " and resid 63   and name HA  ))
  (  segid "BrD " and resid 63   and name HD2%)
     3.300     2.700     2.200 peak  2742 weight  0.11000E+01 volume  0.65439E+02 ppm1     5.296 ppm2     1.490
ASSI { 2752}
  (( segid "BrD " and resid 63   and name HB2 ))
  (  segid "BrD " and resid 63   and name HD1%)
     2.500     1.600     1.600 peak  2752 weight  0.11000E+01 volume  0.34992E+03 ppm1     2.538 ppm2     1.653
ASSI { 2762}
  (( segid "BrD " and resid 63   and name HB2 ))
  (  segid "BrD " and resid 63   and name HD2%)
     2.700     1.800     1.800 peak  2762 weight  0.11000E+01 volume  0.19887E+03 ppm1     2.538 ppm2     1.491
ASSI { 2772}
  (( segid "BrD " and resid 63   and name HB1 ))
  (  segid "BrD " and resid 63   and name HD1%)
     2.600     1.700     1.700 peak  2772 weight  0.11000E+01 volume  0.26127E+03 ppm1     2.883 ppm2     1.653
ASSI { 2782}
  (( segid "BrD " and resid 63   and name HB1 ))
  (  segid "BrD " and resid 63   and name HD2%)
     2.600     1.700     1.700 peak  2782 weight  0.11000E+01 volume  0.25187E+03 ppm1     2.883 ppm2     1.491
ASSI { 2852}
  (  segid "BrD " and resid 14   and name HD2%)
  (( segid "BrD " and resid 14   and name HA  ))
     3.100     2.400     2.400 peak  2852 weight  0.11000E+01 volume  0.89872E+02 ppm1     1.400 ppm2     4.655
ASSI { 2862}
  (  segid "BrD " and resid 14   and name HD2%)
  (( segid "BrD " and resid 14   and name HG  ))
     2.700     1.800     1.800 peak  2862 weight  0.11000E+01 volume  0.20094E+03 ppm1     1.401 ppm2     2.061
ASSI { 2872}
  (( segid "BrD " and resid 24   and name HA  ))
  (( segid "BrD " and resid 24   and name HG1 ))
     2.700     1.800     1.800 peak  2872 weight  0.11000E+01 volume  0.22636E+03 ppm1     4.783 ppm2     3.454
ASSI { 2892}
  (( segid "BrD " and resid 24   and name HG2 ))
  (( segid "BrD " and resid 24   and name HA  ))
     2.400     1.400     1.400 peak  2892 weight  0.11000E+01 volume  0.36992E+03 ppm1     3.076 ppm2     4.784
ASSI { 2902}
  (( segid "BrD " and resid 83   and name HB  ))
  (( segid "BrD " and resid 83   and name HA  ))
     2.300     1.300     1.300 peak  2902 weight  0.11000E+01 volume  0.54241E+03 ppm1     4.804 ppm2     4.460
ASSI { 2912}
  (( segid "BrD " and resid 17   and name HA  ))
  (( segid "BrD " and resid 17   and name HB  ))
     2.500     1.600     1.600 peak  2912 weight  0.11000E+01 volume  0.32083E+03 ppm1     4.562 ppm2     4.860
ASSI { 2932}
  (  segid "BrD " and resid 25   and name HG2%)
  (( segid "BrD " and resid 25   and name HB  ))
     2.300     1.300     1.300 peak  2932 weight  0.11000E+01 volume  0.60381E+03 ppm1     1.650 ppm2     3.005
ASSI { 2942}
  (  segid "BrD " and resid 25   and name HG1%)
  (( segid "BrD " and resid 25   and name HB  ))
     2.200     1.200     1.200 peak  2942 weight  0.11000E+01 volume  0.72430E+03 ppm1     1.795 ppm2     3.006
ASSI { 2972}
  (( segid "BrD " and resid 49   and name HA  ))
  (( segid "BrD " and resid 49   and name HB  ))
     2.500     1.600     1.600 peak  2972 weight  0.11000E+01 volume  0.32061E+03 ppm1     4.658 ppm2     2.620
ASSI { 2992}
  (( segid "BrD " and resid 49   and name HA  ))
  (  segid "BrD " and resid 49   and name HG2%)
     2.900     2.100     2.100 peak  2992 weight  0.11000E+01 volume  0.13480E+03 ppm1     4.658 ppm2     1.870
ASSI { 3012}
  (( segid "BrD " and resid 49   and name HB  ))
  (  segid "BrD " and resid 49   and name HG2%)
     2.500     1.600     1.600 peak  3012 weight  0.11000E+01 volume  0.36520E+03 ppm1     2.634 ppm2     1.570
ASSI { 3022}
  (  segid "BrD " and resid 49   and name HG1%)
  (( segid "BrD " and resid 49   and name HB  ))
     2.500     1.600     1.600 peak  3022 weight  0.11000E+01 volume  0.34642E+03 ppm1     1.647 ppm2     2.615
ASSI { 3042}
  (  segid "BrD " and resid 49   and name HG1%)
  (( segid "BrD " and resid 49   and name HA  ))
     2.700     1.800     1.800 peak  3042 weight  0.11000E+01 volume  0.21850E+03 ppm1     1.647 ppm2     4.679
ASSI { 3052}
  (  segid "BrD " and resid 69   and name HG1%)
  (( segid "BrD " and resid 69   and name HA  ))
     2.100     1.100     1.100 peak  3052 weight  0.11000E+01 volume  0.91954E+03 ppm1     1.550 ppm2     4.695
ASSI { 3072}
  (( segid "BrD " and resid 58   and name HA  ))
  (( segid "BrD " and resid 58   and name HB  ))
     2.200     1.200     1.200 peak  3072 weight  0.11000E+01 volume  0.67241E+03 ppm1     4.456 ppm2     4.703
ASSI { 3102}
  (( segid "BrD " and resid 28   and name HB2 ))
  (( segid "BrD " and resid 28   and name HA  ))
     2.800     2.000     2.000 peak  3102 weight  0.11000E+01 volume  0.15370E+03 ppm1     3.372 ppm2     4.582
ASSI { 3112}
  (( segid "BrD " and resid 28   and name HB1 ))
  (( segid "BrD " and resid 28   and name HA  ))
     2.800     2.000     2.000 peak  3112 weight  0.11000E+01 volume  0.16666E+03 ppm1     3.571 ppm2     4.582
ASSI { 3142}
  (( segid "BrD " and resid 64   and name HA  ))
  (( segid "BrD " and resid 64   and name HD1 ))
     3.000     2.200     2.200 peak  3142 weight  0.11000E+01 volume  0.11363E+03 ppm1     4.950 ppm2     3.393
ASSI { 3162}
  (( segid "BrD " and resid 64   and name HB1 ))
  (( segid "BrD " and resid 64   and name HA  ))
     2.200     1.200     1.200 peak  3162 weight  0.11000E+01 volume  0.77951E+03 ppm1     2.636 ppm2     4.940
ASSI { 3172}
  (( segid "BrD " and resid 64   and name HG1 ))
  (( segid "BrD " and resid 64   and name HA  ))
     2.500     1.600     1.600 peak  3172 weight  0.11000E+01 volume  0.29624E+03 ppm1     2.190 ppm2     4.938
ASSI { 3182}
  (( segid "BrD " and resid 64   and name HG1 ))
  (( segid "BrD " and resid 64   and name HB1 ))
     2.300     1.300     1.300 peak  3182 weight  0.11000E+01 volume  0.60420E+03 ppm1     2.190 ppm2     2.662
ASSI { 3192}
  (( segid "BrD " and resid 64   and name HG1 ))
  (( segid "BrD " and resid 64   and name HE1 ))
     2.500     1.600     1.600 peak  3192 weight  0.11000E+01 volume  0.31904E+03 ppm1     2.190 ppm2     3.897
ASSI { 3202}
  (( segid "BrD " and resid 6    and name HB1 ))
  (( segid "BrD " and resid 6    and name HA  ))
     2.400     1.400     1.400 peak  3202 weight  0.11000E+01 volume  0.45358E+03 ppm1     2.489 ppm2     4.969
ASSI { 3212}
  (( segid "BrD " and resid 6    and name HD1 ))
  (( segid "BrD " and resid 6    and name HA  ))
     2.800     2.000     2.000 peak  3212 weight  0.11000E+01 volume  0.15911E+03 ppm1     2.310 ppm2     4.972
ASSI { 3222}
  (( segid "BrD " and resid 6    and name HG2 ))
  (( segid "BrD " and resid 6    and name HA  ))
     2.900     2.100     2.100 peak  3222 weight  0.11000E+01 volume  0.13404E+03 ppm1     2.040 ppm2     4.973
ASSI { 3232}
  (( segid "BrD " and resid 104  and name HG1 ))
  (( segid "BrD " and resid 104  and name HA  ))
     2.400     1.400     1.400 peak  3232 weight  0.11000E+01 volume  0.41964E+03 ppm1     2.140 ppm2     4.673
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ASSI { 3242}
  (( segid "BrD " and resid 104  and name HA  ))
  (( segid "BrD " and resid 104  and name HB1 ))
    2.100     1.100     1.100 peak  3242 weight  0.11000E+01 volume  0.87442E+03 ppm1      4.657 ppm2      2.537
ASSI { 3272}
  (( segid "BrD " and resid 104  and name HA  ))
  (( segid "BrD " and resid 107  and name HB1 ))
    2.500     1.600     1.600 peak  3272 weight  0.11000E+01 volume  0.31692E+03 ppm1      4.656 ppm2      3.663
ASSI { 3292}
  (( segid "BrD " and resid 111  and name HB2 ))
  (( segid "BrD " and resid 111  and name HA  ))
    2.100     1.100     1.100 peak  3292 weight  0.11000E+01 volume  0.10458E+04 ppm1      2.366 ppm2      4.656
ASSI { 3312}
  (( segid "BrD " and resid 111  and name HA  ))
  (( segid "BrD " and resid 111  and name HG2 ))
    2.800     2.000     2.000 peak  3312 weight  0.11000E+01 volume  0.17232E+03 ppm1      4.656 ppm2      1.918
ASSI { 3332}
  (( segid "BrD " and resid 111  and name HA  ))
  (( segid "BrD " and resid 111  and name HB1 ))
    2.100     1.100     1.100 peak  3332 weight  0.11000E+01 volume  0.97565E+03 ppm1      4.656 ppm2      2.473
ASSI { 3362}
  (( segid "BrD " and resid 19   and name HA  ))
  (( segid "BrD " and resid 19   and name HD1 ))
    3.100     2.400     2.400 peak  3362 weight  0.11000E+01 volume  0.91418E+02 ppm1      4.310 ppm2      2.214
ASSI { 3372}
  (( segid "BrD " and resid 19   and name HB1 ))
  (( segid "BrD " and resid 19   and name HA  ))
    2.500     1.600     1.600 peak  3372 weight  0.11000E+01 volume  0.34161E+03 ppm1      2.290 ppm2      4.297
ASSI { 3382}
  (( segid "BrD " and resid 19   and name HB1 ))
  (( segid "BrD " and resid 16   and name HA  ))
    3.900     3.800     1.600 peak  3382 weight  0.11000E+01 volume  0.22305E+02 ppm1      2.290 ppm2      4.507
ASSI { 3392}
  (( segid "BrD " and resid 19   and name HG1 ))
  (( segid "BrD " and resid 19   and name HA  ))
    2.400     1.400     1.400 peak  3392 weight  0.11000E+01 volume  0.37229E+03 ppm1      1.895 ppm2      4.296
ASSI { 3402}
  (( segid "BrD " and resid 19   and name HG1 ))
  (( segid "BrD " and resid 19   and name HE1 ))
    2.600     1.700     1.700 peak  3402 weight  0.11000E+01 volume  0.28547E+03 ppm1      1.895 ppm2      3.526
ASSI { 3412}
  (( segid "BrD " and resid 19   and name HD1 ))
  (( segid "BrD " and resid 19   and name HE1 ))
    1.800     0.800     0.800 peak  3412 weight  0.11000E+01 volume  0.21730E+04 ppm1      2.192 ppm2      3.522
ASSI { 3422}
  (( segid "BrD " and resid 60   and name HA  ))
  (( segid "BrD " and resid 60   and name HB1 ))
    1.700     0.700     0.700 peak  3422 weight  0.11000E+01 volume  0.29577E+04 ppm1      4.805 ppm2      4.995
ASSI { 3452}
  (( segid "BrD " and resid 11   and name HB1 ))
  (( segid "BrD " and resid 11   and name HA  ))
    2.300     1.300     1.300 peak  3452 weight  0.11000E+01 volume  0.52164E+03 ppm1      2.933 ppm2      4.942
ASSI { 3462}
  (( segid "BrD " and resid 11   and name HB2 ))
  (( segid "BrD " and resid 11   and name HA  ))
    2.300     1.300     1.300 peak  3462 weight  0.11000E+01 volume  0.61125E+03 ppm1      2.586 ppm2      4.943
ASSI { 3492}
  (( segid "BrD " and resid 97   and name HA  ))
  (( segid "BrD " and resid 97   and name HB1 ))
    2.300     1.300     1.300 peak  3492 weight  0.11000E+01 volume  0.52974E+03 ppm1      4.805 ppm2      2.704
ASSI { 3532}
  (( segid "BrD " and resid 109  and name HE2 ))
  (( segid "BrD " and resid 109  and name HD1 ))
    2.500     1.600     1.600 peak  3532 weight  0.11000E+01 volume  0.30326E+03 ppm1      3.029 ppm2      1.994
ASSI { 3542}
  (( segid "BrD " and resid 109  and name HE2 ))
  (( segid "BrD " and resid 109  and name HG1 ))
    2.700     1.800     1.800 peak  3542 weight  0.11000E+01 volume  0.22719E+03 ppm1      3.027 ppm2      1.411
ASSI { 3552}
  (( segid "BrD " and resid 109  and name HE1 ))
  (( segid "BrD " and resid 109  and name HG1 ))
    2.600     1.700     1.700 peak  3552 weight  0.11000E+01 volume  0.23490E+03 ppm1      3.176 ppm2      1.411
ASSI { 3562}
  (( segid "BrD " and resid 109  and name HD1 ))
  (( segid "BrD " and resid 109  and name HE1 ))
    2.700     1.800     1.800 peak  3562 weight  0.11000E+01 volume  0.22693E+03 ppm1      1.994 ppm2      3.195
ASSI { 3602}
  (( segid "BrD " and resid 86   and name HE1 ))
  (( segid "BrD " and resid 86   and name HG2 ))
    2.900     2.100     2.100 peak  3602 weight  0.11000E+01 volume  0.13036E+03 ppm1      3.080 ppm2      0.766
ASSI { 3612}
  (( segid "BrD " and resid 86   and name HD1 ))
  (( segid "BrD " and resid 86   and name HG2 ))
    2.300     1.300     1.300 peak  3612 weight  0.11000E+01 volume  0.49629E+03 ppm1      1.896 ppm2      0.765
ASSI { 3622}
  (( segid "BrD " and resid 86   and name HD1 ))
  (( segid "BrD " and resid 86   and name HE1 ))
    2.600     1.700     1.700 peak  3622 weight  0.11000E+01 volume  0.24556E+03 ppm1      1.892 ppm2      3.093
ASSI { 3632}
  (( segid "BrD " and resid 86   and name HA  ))
  (( segid "BrD " and resid 86   and name HG1 ))
    2.800     2.000     2.000 peak  3632 weight  0.11000E+01 volume  0.14893E+03 ppm1      4.806 ppm2      1.895
ASSI { 3682}
  (( segid "BrD " and resid 8    and name HG1 ))
  (( segid "BrD " and resid 8    and name HD1 ))
    2.000     1.000     1.000 peak  3682 weight  0.11000E+01 volume  0.11498E+04 ppm1      2.635 ppm2      4.436
ASSI { 3692}
  (( segid "BrD " and resid 8    and name HG1 ))
  (( segid "BrD " and resid 8    and name HD2 ))
    2.100     1.100     1.100 peak  3692 weight  0.11000E+01 volume  0.87712E+03 ppm1      2.635 ppm2      4.286
ASSI { 3702}
  (( segid "BrD " and resid 8    and name HB2 ))
  (( segid "BrD " and resid 8    and name HA  ))
    2.600     1.700     1.700 peak  3702 weight  0.11000E+01 volume  0.24482E+03 ppm1      2.487 ppm2      5.021
ASSI { 3712}
  (( segid "BrD " and resid 8    and name HB1 ))
  (( segid "BrD " and resid 8    and name HA  ))
    2.400     1.400     1.400 peak  3712 weight  0.11000E+01 volume  0.36862E+03 ppm1      2.831 ppm2      5.021
ASSI { 3722}
  (( segid "BrD " and resid 8    and name HD1 ))
  (( segid "BrD " and resid 7    and name HA  ))
    2.100     1.100     1.100 peak  3722 weight  0.11000E+01 volume  0.89203E+03 ppm1      4.407 ppm2      5.144
ASSI { 3732}
  (( segid "BrD " and resid 8    and name HD1 ))
  (( segid "BrD " and resid 7    and name HA  ))
    2.100     1.100     1.100 peak  3732 weight  0.11000E+01 volume  0.93259E+03 ppm1      4.263 ppm2      5.144
ASSI { 3752}
  (( segid "BrD " and resid 44   and name HA  ))
  (( segid "BrD " and resid 44   and name HB1 ))
    2.400     1.400     1.400 peak  3752 weight  0.11000E+01 volume  0.42716E+03 ppm1      5.098 ppm2      2.973
ASSI { 3762}
  (( segid "BrD " and resid 44   and name HA  ))
  (( segid "BrD " and resid 44   and name HB2 ))
    2.600     1.700     1.700 peak  3762 weight  0.11000E+01 volume  0.27521E+03 ppm1      5.098 ppm2      2.636
ASSI { 3792}
  (( segid "BrD " and resid 44   and name HB2 ))
  (( segid "BrD " and resid 44   and name HD1 ))
    2.800     2.000     2.000 peak  3792 weight  0.11000E+01 volume  0.16780E+03 ppm1      2.631 ppm2      4.337
ASSI { 3802}
  (( segid "BrD " and resid 44   and name HB1 ))
  (( segid "BrD " and resid 44   and name HD1 ))
    3.200     2.600     2.300 peak  3802 weight  0.11000E+01 volume  0.70033E+02 ppm1      2.981 ppm2      4.337
ASSI { 3822}
  (( segid "BrD " and resid 44   and name HG1 ))
  (( segid "BrD " and resid 44   and name HA  ))
    2.900     2.100     2.100 peak  3822 weight  0.11000E+01 volume  0.14259E+03 ppm1      2.729 ppm2      5.114
ASSI { 3832}
  (( segid "BrD " and resid 44   and name HG2 ))
  (( segid "BrD " and resid 44   and name HA  ))
    2.700     1.800     1.800 peak  3832 weight  0.11000E+01 volume  0.22601E+03 ppm1      2.665 ppm2      5.114
ASSI { 3842}
  (( segid "BrD " and resid 41   and name HA  ))
  (( segid "BrD " and resid 41   and name HB  ))
    1.900     0.900     0.900 peak  3842 weight  0.11000E+01 volume  0.19310E+04 ppm1      4.657 ppm2      4.899
ASSI { 3882}
  (( segid "BrD " and resid 103  and name HG2 ))
  (( segid "BrD " and resid 103  and name HA  ))
    2.800     2.000     2.000 peak  3882 weight  0.11000E+01 volume  0.14970E+03 ppm1      2.519 ppm2      3.789
ASSI { 3892}
  (( segid "BrD " and resid 103  and name HG1 ))
  (( segid "BrD " and resid 103  and name HA  ))
    2.900     2.100     2.100 peak  3892 weight  0.11000E+01 volume  0.14619E+03 ppm1      2.598 ppm2      3.789
ASSI { 3912}
  (( segid "BrD " and resid 103  and name HG2 ))
  (( segid "BrD " and resid 103  and name HB1 ))
    3.000     3.200     2.200 peak  3912 weight  0.11000E+01 volume  0.10661E+03 ppm1      2.519 ppm2      2.346
ASSI { 3922}
  (( segid "BrD " and resid 103  and name HG1 ))
  (( segid "BrD " and resid 103  and name HB1 ))
    3.200     2.600     2.300 peak  3922 weight  0.11000E+01 volume  0.80668E+02 ppm1      2.598 ppm2      2.346
ASSI { 3942}
  (( segid "BrD " and resid 48   and name HA  ))
  (( segid "BrD " and resid 48   and name HG1 ))
    3.100     2.400     2.400 peak  3942 weight  0.11000E+01 volume  0.93117E+02 ppm1      4.803 ppm2      2.940
ASSI { 3952}
  (( segid "BrD " and resid 48   and name HA  ))
  (( segid "BrD " and resid 48   and name HG2 ))
    3.000     2.200     2.200 peak  3952 weight  0.11000E+01 volume  0.10971E+03 ppm1      4.803 ppm2      2.851
ASSI { 3982}
  (  segid "BrD " and resid 50   and name HD1%)
  (( segid "BrD " and resid 50   and name HA  ))
    2.300     1.300     1.300 peak  3982 weight  0.11000E+01 volume  0.51678E+03 ppm1      1.155 ppm2      4.518
ASSI { 4012}
  (  segid "BrD " and resid 110  and name HD1%)
  (( segid "BrD " and resid 110  and name HG12))
    2.600     1.700     1.700 peak  4012 weight  0.11000E+01 volume  0.27804E+03 ppm1      1.154 ppm2      1.652
ASSI { 4022}
  (  segid "BrD " and resid 110  and name HG2%)
  (( segid "BrD " and resid 110  and name HG12))
    2.500     1.600     1.600 peak  4022 weight  0.11000E+01 volume  0.35399E+03 ppm1      1.253 ppm2      1.651
ASSI { 4032}
  (( segid "BrD " and resid 110  and name HB  ))
  (( segid "BrD " and resid 110  and name HG12))
    3.300     2.700     2.300 peak  4032 weight  0.11000E+01 volume  0.60399E+02 ppm1      2.330 ppm2      1.651
ASSI { 4052}
  (( segid "BrD " and resid 24   and name HB1 ))
  (( segid "BrD " and resid 24   and name HG1 ))
    2.600     1.700     1.700 peak  4052 weight  0.11000E+01 volume  0.27715E+03 ppm1      3.076 ppm2      3.453
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ASSI ( 4062)
   (( segid "BrD " and resid 80   and name HD1 ))
   (( segid "BrD " and resid 80   and name HG1 ))
      2.400     1.400     1.400 peak  4062 weight  0.11000E+01 volume  0.37330E+03 ppm1     3.956 ppm2     2.347
ASSI ( 4072)
   (( segid "BrD " and resid 80   and name HD1 ))
   (( segid "BrD " and resid 80   and name HB1 ))
      2.700     1.800     1.800 peak  4072 weight  0.11000E+01 volume  0.22342E+03 ppm1     3.956 ppm2     2.573
ASSI ( 4112)
   (( segid "BrD " and resid 101  and name HA  ))
   (( segid "BrD " and resid 101  and name HB  ))
      2.600     1.700     1.700 peak  4112 weight  0.11000E+01 volume  0.25152E+03 ppm1     4.263 ppm2     2.535
ASSI ( 4122)
   (( segid "BrD " and resid 101  and name HA  ))
   (( segid "BrD " and resid 101  and name HG11))
      2.600     1.700     1.700 peak  4122 weight  0.11000E+01 volume  0.23036E+03 ppm1     4.263 ppm2     2.469
ASSI ( 4132)
   (( segid "BrD " and resid 101  and name HA  ))
   (( segid "BrD " and resid 101  and name HG12))
      2.500     1.600     1.600 peak  4132 weight  0.11000E+01 volume  0.31941E+03 ppm1     4.261 ppm2     1.806
ASSI ( 4142)
   (  segid "BrD " and resid 38   and name HG1%)
   (( segid "BrD " and resid 38   and name HA  ))
      2.300     1.300     1.300 peak  4142 weight  0.11000E+01 volume  0.50426E+03 ppm1     1.058 ppm2     4.168
ASSI ( 4162)
   (  segid "BrD " and resid 81   and name HG2%)
   (( segid "BrD " and resid 81   and name HA  ))
      2.400     1.400     1.400 peak  4162 weight  0.11000E+01 volume  0.38926E+03 ppm1     0.761 ppm2     3.716
ASSI ( 4182)
   (  segid "BrD " and resid 81   and name HG1%)
   (( segid "BrD " and resid 81   and name HA  ))
      2.400     1.400     1.400 peak  4182 weight  0.11000E+01 volume  0.43696E+03 ppm1     1.059 ppm2     3.716
ASSI ( 4212)
   (( segid "BrD " and resid 69   and name HB  ))
   (( segid "BrD " and resid 69   and name HA  ))
      2.200     1.200     1.200 peak  4212 weight  0.11000E+01 volume  0.67869E+03 ppm1     2.929 ppm2     4.696
ASSI ( 4222)
   (( segid "BrD " and resid 18   and name HA  ))
   (( segid "BrD " and resid 18   and name HB1 ))
      2.800     2.000     2.000 peak  4222 weight  0.11000E+01 volume  0.15123E+03 ppm1     3.666 ppm2     2.131
ASSI ( 4272)
   (( segid "BrD " and resid 116  and name HB  ))
   (  segid "BrD " and resid 116  and name HD1%)
      2.500     1.600     1.600 peak  4272 weight  0.11000E+01 volume  0.31982E+03 ppm1     2.409 ppm2     1.399
ASSI ( 4282)
   (( segid "BrD " and resid 110  and name HB  ))
   (( segid "BrD " and resid 110  and name HG11))
      3.100     2.400     2.400 peak  4282 weight  0.11000E+01 volume  0.90397E+02 ppm1     2.338 ppm2     1.718
ASSI ( 4302)
   (( segid "BrD " and resid 50   and name HA  ))
   (( segid "BrD " and resid 50   and name HG11))
      2.600     1.700     1.700 peak  4302 weight  0.11000E+01 volume  0.24102E+03 ppm1     4.506 ppm2     1.409
ASSI ( 4322)
   (( segid "BrD " and resid 50   and name HB  ))
   (( segid "BrD " and resid 50   and name HG12))
      2.700     1.800     1.800 peak  4322 weight  0.11000E+01 volume  0.20938E+03 ppm1     1.797 ppm2     0.840
ASSI ( 4332)
   (( segid "BrD " and resid 50   and name HB  ))
   (( segid "BrD " and resid 50   and name HG11))
      2.700     1.800     1.800 peak  4332 weight  0.11000E+01 volume  0.20876E+03 ppm1     1.797 ppm2     1.407
ASSI ( 4342)
   (( segid "BrD " and resid 50   and name HB  ))
   (( segid "BrD " and resid 50   and name HA  ))
      3.000     2.200     2.200 peak  4342 weight  0.11000E+01 volume  0.11875E+03 ppm1     1.797 ppm2     4.516
ASSI ( 4382)
   (( segid "BrD " and resid 21   and name HA  ))
   (( segid "BrD " and resid 21   and name HB  ))
      2.700     1.800     1.800 peak  4382 weight  0.11000E+01 volume  0.19816E+03 ppm1     4.359 ppm2     2.515
ASSI ( 4392)
   (( segid "BrD " and resid 21   and name HA  ))
   (( segid "BrD " and resid 21   and name HG12))
      2.600     1.700     1.700 peak  4392 weight  0.11000E+01 volume  0.25295E+03 ppm1     4.358 ppm2     1.653
ASSI ( 4402)
   (( segid "BrD " and resid 21   and name HA  ))
   (( segid "BrD " and resid 21   and name HG11))
      2.600     1.700     1.700 peak  4402 weight  0.11000E+01 volume  0.24995E+03 ppm1     4.358 ppm2     2.357
ASSI ( 4412)
   (( segid "BrD " and resid 21   and name HB  ))
   (( segid "BrD " and resid 21   and name HG11))
      2.900     2.100     2.100 peak  4412 weight  0.11000E+01 volume  0.13199E+03 ppm1     2.487 ppm2     2.356
ASSI ( 4472)
   (( segid "BrD " and resid 21   and name HG12))
   (( segid "BrD " and resid 21   and name HB  ))
      2.800     2.000     2.000 peak  4472 weight  0.11000E+01 volume  0.17027E+03 ppm1     1.642 ppm2     2.511
ASSI ( 4482)
   (( segid "BrD " and resid 21   and name HG12))
   (( segid "BrD " and resid 21   and name HG11))
      2.200     1.200     1.200 peak  4482 weight  0.11000E+01 volume  0.65087E+03 ppm1     1.642 ppm2     2.357
ASSI ( 4502)
   (  segid "BrD " and resid 21   and name HG2%)
   (( segid "BrD " and resid 21   and name HA  ))
      2.400     1.400     1.400 peak  4502 weight  0.11000E+01 volume  0.39582E+03 ppm1     1.596 ppm2     4.369
ASSI ( 4512)
   (( segid "BrD " and resid 36   and name HG1 ))
   (( segid "BrD " and resid 36   and name HB2 ))
      2.100     1.100     1.100 peak  4512 weight  0.11000E+01 volume  0.10618E+04 ppm1     2.781 ppm2     2.342
ASSI ( 4562)
   (( segid "BrD " and resid 9    and name HG1 ))
   (( segid "BrD " and resid 9    and name HA  ))
      2.800     2.000     2.000 peak  4562 weight  0.11000E+01 volume  0.15274E+03 ppm1     2.236 ppm2     4.940
ASSI ( 4582)
   (( segid "BrD " and resid 9    and name HA  ))
   (( segid "BrD " and resid 9    and name HB2 ))
      2.400     1.400     1.400 peak  4582 weight  0.11000E+01 volume  0.39636E+03 ppm1     4.953 ppm2     2.385
ASSI ( 4592)
   (( segid "BrD " and resid 35   and name HB2 ))
   (( segid "BrD " and resid 35   and name HG1 ))
      2.600     1.700     1.700 peak  4592 weight  0.11000E+01 volume  0.27554E+03 ppm1     2.781 ppm2     3.447
ASSI ( 4602)
   (( segid "BrD " and resid 35   and name HB1 ))
   (( segid "BrD " and resid 35   and name HG1 ))
      3.000     2.200     2.200 peak  4602 weight  0.11000E+01 volume  0.10522E+03 ppm1     2.838 ppm2     3.447
ASSI ( 4632)
   (  segid "BrD " and resid 73   and name HD1%)
   (( segid "BrD " and resid 73   and name HG  ))
      2.100     1.100     1.100 peak  4632 weight  0.11000E+01 volume  0.81939E+03 ppm1     1.549 ppm2     2.368
ASSI ( 4642)
   (( segid "BrD " and resid 56   and name HA  ))
   (( segid "BrD " and resid 56   and name HB1 ))
      2.500     1.600     1.600 peak  4642 weight  0.11000E+01 volume  0.31507E+03 ppm1     4.606 ppm2     2.694
ASSI ( 4652)
   (  segid "BrD " and resid 22   and name HD2%)
   (( segid "BrD " and resid 22   and name HB1 ))
      2.500     1.600     1.600 peak  4652 weight  0.11000E+01 volume  0.35307E+03 ppm1     1.600 ppm2     3.702
ASSI ( 4662)
   (( segid "BrD " and resid 22   and name HA  ))
   (( segid "BrD " and resid 22   and name HG  ))
      2.400     1.400     1.400 peak  4662 weight  0.11000E+01 volume  0.43065E+03 ppm1     4.704 ppm2     2.360
ASSI ( 4722)
   (( segid "BrD " and resid 14   and name HA  ))
   (( segid "BrD " and resid 14   and name HB1 ))
      2.400     1.400     1.400 peak  4722 weight  0.11000E+01 volume  0.40350E+03 ppm1     4.655 ppm2     2.464
ASSI ( 4732)
   (( segid "BrD " and resid 14   and name HA  ))
   (( segid "BrD " and resid 14   and name HB2 ))
      2.500     1.600     1.600 peak  4732 weight  0.11000E+01 volume  0.34201E+03 ppm1     4.655 ppm2     2.159
ASSI ( 4742)
   (( segid "BrD " and resid 14   and name HA  ))
   (( segid "BrD " and resid 14   and name HG  ))
      2.800     2.000     2.000 peak  4742 weight  0.11000E+01 volume  0.16298E+03 ppm1     4.655 ppm2     2.062
ASSI ( 4752)
   (  segid "BrD " and resid 14   and name HD2%)
   (( segid "BrD " and resid 14   and name HB2 ))
      2.900     2.100     2.100 peak  4752 weight  0.11000E+01 volume  0.12176E+03 ppm1     1.401 ppm2     2.155
ASSI ( 4762)
   (  segid "BrD " and resid 14   and name HD2%)
   (( segid "BrD " and resid 14   and name HB1 ))
      2.200     1.200     1.200 peak  4762 weight  0.11000E+01 volume  0.78049E+03 ppm1     1.401 ppm2     2.466
ASSI ( 4782)
   (( segid "BrD " and resid 24   and name HB2 ))
   (( segid "BrD " and resid 24   and name HG1 ))
      2.700     1.800     1.800 peak  4782 weight  0.11000E+01 volume  0.20235E+03 ppm1     2.989 ppm2     3.453
ASSI ( 4812)
   (( segid "BrD " and resid 25   and name HA  ))
   (  segid "BrD " and resid 25   and name HG2%)
      2.400     1.700     1.700 peak  4812 weight  0.11000E+01 volume  0.28433E+03 ppm1     4.412 ppm2     1.637
ASSI ( 4822)
   (  segid "BrD " and resid 25   and name HG1%)
   (( segid "BrD " and resid 25   and name HA  ))
      2.300     1.300     1.300 peak  4822 weight  0.11000E+01 volume  0.50491E+03 ppm1     1.796 ppm2     4.427
ASSI ( 4832)
   (( segid "BrD " and resid 30   and name HB1 ))
   (( segid "BrD " and resid 30   and name HA  ))
      2.700     1.800     1.800 peak  4832 weight  0.11000E+01 volume  0.18839E+03 ppm1     4.907 ppm2     5.445
ASSI ( 4852)
   (( segid "BrD " and resid 30   and name HA  ))
   (( segid "BrD " and resid 30   and name HB2 ))
      2.900     2.100     2.100 peak  4852 weight  0.11000E+01 volume  0.13612E+03 ppm1     5.444 ppm2     4.533
ASSI ( 4862)
   (( segid "BrD " and resid 104  and name HE1 ))
   (( segid "BrD " and resid 104  and name HD1 ))
      1.900     0.900     0.900 peak  4862 weight  0.11000E+01 volume  0.17529E+04 ppm1     3.571 ppm2     2.290
ASSI ( 4912)
   (( segid "BrD " and resid 57   and name HG1 ))
   (( segid "BrD " and resid 57   and name HA  ))
      2.400     1.400     1.400 peak  4912 weight  0.11000E+01 volume  0.42230E+03 ppm1     2.110 ppm2     4.800
ASSI ( 4922)
   (( segid "BrD " and resid 57   and name HE1 ))
   (( segid "BrD " and resid 57   and name HG2 ))
      2.200     1.200     1.200 peak  4922 weight  0.11000E+01 volume  0.69710E+03 ppm1     3.569 ppm2     2.172
ASSI ( 4932)
   (( segid "BrD " and resid 109  and name HA  ))
   (( segid "BrD " and resid 109  and name HB2 ))
      2.000     1.000     1.000 peak  4932 weight  0.11000E+01 volume  0.10760E+04 ppm1     4.653 ppm2     2.149
ASSI ( 4942)
   (( segid "BrD " and resid 109  and name HA  ))
   (( segid "BrD " and resid 109  and name HB1 ))
      2.000     1.000     1.000 peak  4942 weight  0.11000E+01 volume  0.13416E+04 ppm1     4.653 ppm2     2.321
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ASSI ( 4962)
   (( segid "BrD " and resid 109  and name HB2 ))
   (( segid "BrD " and resid 109  and name HQ1 ))
     2.500     1.600     1.600 peak  4962 weight  0.11000E+01 volume  0.29632E+03 ppm1      2.141 ppm2      1.417
ASSI ( 4972)
   (( segid "BrD " and resid 109  and name HB1 ))
   (( segid "BrD " and resid 109  and name HQ1 ))
     2.500     1.600     1.600 peak  4972 weight  0.11000E+01 volume  0.36408E+03 ppm1      2.334 ppm2      1.417
ASSI ( 4982)
   (( segid "BrD " and resid 109  and name HQ1 ))
   (( segid "BrD " and resid 109  and name HA  ))
     2.700     1.800     1.800 peak  4982 weight  0.11000E+01 volume  0.22259E+03 ppm1      1.399 ppm2      4.639
ASSI ( 5002)
   (( segid "BrD " and resid 109  and name HE2 ))
   (( segid "BrD " and resid 109  and name HA  ))
     2.800     2.000     2.000 peak  5002 weight  0.11000E+01 volume  0.16510E+03 ppm1      3.029 ppm2      4.639
ASSI ( 5012)
   (( segid "BrD " and resid 86   and name HQ2 ))
   (( segid "BrD " and resid 86   and name HA  ))
     2.800     2.000     2.000 peak  5012 weight  0.11000E+01 volume  0.18063E+03 ppm1      0.761 ppm2      4.812
ASSI ( 5022)
   (  segid "BrD " and resid 41   and name HQ2%)
   (( segid "BrD " and resid 41   and name HA  ))
     2.200     1.200     1.200 peak  5022 weight  0.11000E+01 volume  0.76022E+03 ppm1      1.844 ppm2      4.671
ASSI ( 5032)
   (  segid "BrD " and resid 41   and name HQ2%)
   (( segid "BrD " and resid 41   and name HB  ))
     2.000     1.000     1.000 peak  5032 weight  0.11000E+01 volume  0.12138E+04 ppm1      1.845 ppm2      4.901
ASSI ( 5042)
   (  segid "BrD " and resid 58   and name HQ2%)
   (( segid "BrD " and resid 58   and name HA  ))
     2.000     1.000     1.000 peak  5042 weight  0.11000E+01 volume  0.10840E+04 ppm1      1.649 ppm2      4.451
ASSI ( 5052)
   (  segid "BrD " and resid 58   and name HQ2%)
   (( segid "BrD " and resid 58   and name HB  ))
     1.900     0.900     0.900 peak  5052 weight  0.11000E+01 volume  0.14547E+04 ppm1      1.649 ppm2      4.705
ASSI ( 5062)
   (  segid "BrD " and resid 17   and name HQ2%)
   (( segid "BrD " and resid 17   and name HA  ))
     2.300     1.300     1.300 peak  5062 weight  0.11000E+01 volume  0.54601E+03 ppm1      1.747 ppm2      4.542
ASSI ( 5072)
   (  segid "BrD " and resid 17   and name HQ2%)
   (( segid "BrD " and resid 17   and name HB  ))
     2.100     1.100     1.100 peak  5072 weight  0.11000E+01 volume  0.92706E+03 ppm1      1.745 ppm2      4.861
ASSI ( 5082)
   (  segid "BrD " and resid 83   and name HQ2%)
   (( segid "BrD " and resid 83   and name HB  ))
     2.100     1.100     1.100 peak  5082 weight  0.11000E+01 volume  0.10099E+04 ppm1      1.893 ppm2      4.805
ASSI ( 5092)
   (  segid "BrD " and resid 83   and name HQ2%)
   (( segid "BrD " and resid 83   and name HA  ))
     2.200     1.200     1.200 peak  5092 weight  0.11000E+01 volume  0.64890E+03 ppm1      1.894 ppm2      4.460
ASSI ( 5122)
   (( segid "BrD " and resid 37   and name HA  ))
   (( segid "BrD " and resid 37   and name HQ1 ))
     2.800     2.000     2.000 peak  5122 weight  0.11000E+01 volume  0.14935E+03 ppm1      4.853 ppm2      2.725
ASSI ( 5132)
   (( segid "BrD " and resid 37   and name HA  ))
   (( segid "BrD " and resid 37   and name HQ2 ))
     3.200     2.600     2.300 peak  5132 weight  0.11000E+01 volume  0.80336E+02 ppm1      4.853 ppm2      2.587
ASSI ( 5162)
   (( segid "BrD " and resid 37   and name HQ2 ))
   (( segid "BrD " and resid 37   and name HD1 ))
     2.300     1.300     1.300 peak  5162 weight  0.11000E+01 volume  0.49428E+03 ppm1      2.585 ppm2      4.291
ASSI ( 5172)
   (( segid "BrD " and resid 37   and name HQ1 ))
   (( segid "BrD " and resid 37   and name HD1 ))
     2.500     1.600     1.600 peak  5172 weight  0.11000E+01 volume  0.34945E+03 ppm1      2.733 ppm2      4.290
ASSI ( 5182)
   (( segid "BrD " and resid 37   and name HQ1 ))
   (( segid "BrD " and resid 37   and name HB1 ))
     2.300     1.300     1.300 peak  5182 weight  0.11000E+01 volume  0.51291E+03 ppm1      2.733 ppm2      2.961
ASSI ( 5192)
   (( segid "BrD " and resid 37   and name HQ2 ))
   (( segid "BrD " and resid 37   and name HB1 ))
     2.300     1.300     1.300 peak  5192 weight  0.11000E+01 volume  0.56233E+03 ppm1      2.584 ppm2      2.961
ASSI ( 5202)
   (( segid "BrD " and resid 37   and name HB1 ))
   (( segid "BrD " and resid 37   and name HA  ))
     2.200     1.200     1.200 peak  5202 weight  0.11000E+01 volume  0.64791E+03 ppm1      2.935 ppm2      4.858
ASSI ( 5212)
   (( segid "BrD " and resid 37   and name HB2 ))
   (( segid "BrD " and resid 37   and name HA  ))
     2.400     1.400     1.400 peak  5212 weight  0.11000E+01 volume  0.38936E+03 ppm1      2.290 ppm2      4.858
ASSI ( 5222)
   (( segid "BrD " and resid 37   and name HB1 ))
   (( segid "BrD " and resid 37   and name HD1 ))
     1.600     1.200     1.900 peak  5222 weight  0.11000E+01 volume  0.35025E+02 ppm1      2.935 ppm2      4.298
ASSI ( 5272)
   (( segid "BrD " and resid 51   and name HD1 ))
   (( segid "BrD " and resid 52   and name HA  ))
     1.300     2.700     2.200 peak  5272 weight  0.11000E+01 volume  0.68484E+02 ppm1      4.214 ppm1      5.584
ASSI ( 5282)
   (( segid "BrD " and resid 53   and name HB1 ))
   (( segid "BrD " and resid 53   and name HA  ))
     2.200     1.200     1.200 peak  5282 weight  0.11000E+01 volume  0.77735E+03 ppm1      2.760 ppm2      4.686
ASSI ( 5292)
   (( segid "BrD " and resid 53   and name HQ2 ))
   (( segid "BrD " and resid 53   and name HA  ))
     2.900     2.100     2.100 peak  5292 weight  0.11000E+01 volume  0.13643E+03 ppm1      2.487 ppm2      4.687
ASSI ( 5302)
   (( segid "BrD " and resid 51   and name HA  ))
   (( segid "BrD " and resid 51   and name HQ2 ))
     2.300     1.300     1.300 peak  5302 weight  0.11000E+01 volume  0.54723E+03 ppm1      4.459 ppm2      1.786
ASSI ( 5312)
   (( segid "BrD " and resid 51   and name HA  ))
   (( segid "BrD " and resid 51   and name HQ1 ))
     2.400     1.400     1.400 peak  5312 weight  0.11000E+01 volume  0.38819E+03 ppm1      4.459 ppm2      1.946
ASSI ( 5332)
   (( segid "BrD " and resid 51   and name HB1 ))
   (( segid "BrD " and resid 51   and name HA  ))
     2.700     1.800     1.800 peak  5332 weight  0.11000E+01 volume  0.20757E+03 ppm1      1.945 ppm2      4.468
ASSI ( 5342)
   (( segid "BrD " and resid 51   and name HB2 ))
   (( segid "BrD " and resid 51   and name HA  ))
     2.400     1.400     1.400 peak  5342 weight  0.11000E+01 volume  0.37628E+03 ppm1      1.795 ppm2      4.468
ASSI ( 5372)
   (( segid "BrD " and resid 51   and name HQ1 ))
   (( segid "BrD " and resid 51   and name HD1 ))
     2.800     2.000     2.000 peak  5372 weight  0.11000E+01 volume  0.16452E+03 ppm1      1.946 ppm2      3.606
ASSI ( 5382)
   (( segid "BrD " and resid 51   and name HQ2 ))
   (( segid "BrD " and resid 51   and name HD1 ))
     2.400     1.400     1.400 peak  5382 weight  0.11000E+01 volume  0.40668E+03 ppm1      1.796 ppm2      3.606
ASSI ( 5392)
   (( segid "BrD " and resid 51   and name HD1 ))
   (( segid "BrD " and resid 51   and name HB1 ))
     2.500     1.600     1.600 peak  5392 weight  0.11000E+01 volume  0.36659E+03 ppm1      3.577 ppm2      1.945
ASSI ( 5402)
   (( segid "BrD " and resid 51   and name HD1 ))
   (( segid "BrD " and resid 51   and name HB2 ))
     2.400     1.400     1.400 peak  5402 weight  0.11000E+01 volume  0.38417E+03 ppm1      3.577 ppm2      1.795
ASSI ( 5412)
   (( segid "BrD " and resid 51   and name HD1 ))
   (( segid "BrD " and resid 51   and name HA  ))
     2.700     1.800     1.800 peak  5412 weight  0.11000E+01 volume  0.20141E+03 ppm1      3.578 ppm2      4.463
ASSI ( 5422)
   (( segid "BrD " and resid 52   and name HA  ))
   (( segid "BrD " and resid 52   and name HB1 ))
     2.500     1.600     1.600 peak  5422 weight  0.11000E+01 volume  0.31170E+03 ppm1      5.592 ppm2      3.656
ASSI ( 5432)
   (( segid "BrD " and resid 52   and name HA  ))
   (( segid "BrD " and resid 52   and name HB2 ))
     2.800     2.000     2.000 peak  5432 weight  0.11000E+01 volume  0.16779E+03 ppm1      5.593 ppm2      3.533
ASSI ( 5462)
   (( segid "BrD " and resid 75   and name HQ2 ))
   (( segid "BrD " and resid 75   and name HA  ))
     2.700     1.800     1.800 peak  5462 weight  0.11000E+01 volume  0.19830E+03 ppm1      3.226 ppm2      4.517
ASSI ( 5482)
   (( segid "BrD " and resid 75   and name HQ2 ))
   (( segid "BrD " and resid 75   and name HB2 ))
     2.600     1.700     1.700 peak  5482 weight  0.11000E+01 volume  0.27353E+03 ppm1      3.227 ppm2      2.847
ASSI ( 5492)
   (( segid "BrD " and resid 75   and name HQ1 ))
   (( segid "BrD " and resid 75   and name HB2 ))
     2.300     1.300     1.300 peak  5492 weight  0.11000E+01 volume  0.48028E+03 ppm1      3.523 ppm2      2.847
ASSI ( 5502)
   (( segid "BrD " and resid 75   and name HQ1 ))
   (( segid "BrD " and resid 75   and name HB1 ))
     2.700     1.800     1.800 peak  5502 weight  0.11000E+01 volume  0.21586E+03 ppm1      3.523 ppm2      2.931
ASSI ( 5512)
   (( segid "BrD " and resid 75   and name HQ2 ))
   (( segid "BrD " and resid 75   and name HB1 ))
     2.700     1.800     1.800 peak  5512 weight  0.11000E+01 volume  0.21836E+03 ppm1      3.227 ppm2      2.931
ASSI ( 5522)
   (( segid "BrD " and resid 75   and name HA  ))
   (( segid "BrD " and resid 75   and name HQ1 ))
     2.800     2.000     2.000 peak  5522 weight  0.11000E+01 volume  0.16121E+03 ppm1      4.509 ppm2      3.530
ASSI ( 5542)
   (( segid "BrD " and resid 19   and name HB2 ))
   (( segid "BrD " and resid 16   and name HA  ))
     2.900     2.100     2.100 peak  5542 weight  0.11000E+01 volume  0.12463E+03 ppm1      1.989 ppm2      4.907
ASSI ( 5552)
   (( segid "BrD " and resid 19   and name HB2 ))
   (( segid "BrD " and resid 19   and name HA  ))
     2.600     1.700     1.700 peak  5552 weight  0.11000E+01 volume  0.27005E+03 ppm1      1.989 ppm2      4.297
ASSI ( 5582)
   (( segid "BrD " and resid 54   and name HA  ))
   (( segid "BrD " and resid 54   and name HB2 ))
     3.000     2.200     2.200 peak  5582 weight  0.11000E+01 volume  0.10290E+03 ppm1      5.543 ppm2      1.964
ASSI ( 5592)
   (( segid "BrD " and resid 97   and name HQ1 ))
   (( segid "BrD " and resid 97   and name HE1 ))
     3.100     2.400     2.400 peak  5592 weight  0.11000E+01 volume  0.89029E+02 ppm1      2.436 ppm2      3.572
ASSI ( 5622)
   (( segid "BrD " and resid 89   and name HQ2 ))
   (( segid "BrD " and resid 89   and name HA  ))
     2.400     1.400     1.400 peak  5622 weight  0.11000E+01 volume  0.39102E+03 ppm1      3.137 ppm2      4.911
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ASSI ( 5632)
  (( segid "BrD " and resid 59   and name HG1 ))
  (( segid "BrD " and resid 59   and name HA  ))
    3.000     2.200     2.200 peak  5632 weight  0.11000E+01 volume  0.11482E+03 ppm1     3.228 ppm2     4.911
ASSI ( 5642)
  (( segid "BrD " and resid 13   and name HG2 ))
  (( segid "BrD " and resid 13   and name HA  ))
    2.300     1.300     1.300 peak  5642 weight  0.11000E+01 volume  0.56353E+03 ppm1     2.978 ppm2     4.775
ASSI ( 5652)
  (( segid "BrD " and resid 13   and name HG1 ))
  (( segid "BrD " and resid 13   and name HA  ))
    2.800     2.000     2.000 peak  5652 weight  0.11000E+01 volume  0.18150E+03 ppm1     3.131 ppm2     4.775
ASSI ( 5672)
  (( segid "BrD " and resid 57   and name HA  ))
  (( segid "BrD " and resid 57   and name HD1 ))
    2.600     1.700     1.700 peak  5672 weight  0.11000E+01 volume  0.27608E+03 ppm1     4.805 ppm2     2.387
ASSI ( 5682)
  (( segid "BrD " and resid 57   and name HA  ))
  (( segid "BrD " and resid 57   and name HG2 ))
    2.900     2.100     2.100 peak  5682 weight  0.11000E+01 volume  0.12195E+03 ppm1     4.805 ppm2     2.016
ASSI ( 5712)
  (( segid "BrD " and resid 57   and name HB2 ))
  (( segid "BrD " and resid 57   and name HA  ))
    2.500     1.600     1.600 peak  5712 weight  0.11000E+01 volume  0.35277E+03 ppm1     2.843 ppm2     4.800
ASSI ( 5722)
  (( segid "BrD " and resid 57   and name HB1 ))
  (( segid "BrD " and resid 57   and name HA  ))
    2.400     1.400     1.400 peak  5722 weight  0.11000E+01 volume  0.42344E+03 ppm1     2.935 ppm2     4.798
ASSI ( 5732)
  (( segid "BrD " and resid 57   and name HE1 ))
  (( segid "BrD " and resid 57   and name HG2 ))
    2.200     1.300     1.200 peak  5732 weight  0.11000E+01 volume  0.67766E+03 ppm1     3.572 ppm2     2.017
ASSI ( 5752)
  (( segid "BrD " and resid 57   and name HD2 ))
  (( segid "BrD " and resid 57   and name HA  ))
    2.600     1.700     1.700 peak  5752 weight  0.11000E+01 volume  0.24171E+03 ppm1     2.295 ppm2     4.800
ASSI ( 5762)
  (( segid "BrD " and resid 57   and name HD1 ))
  (( segid "BrD " and resid 57   and name HE1 ))
    2.100     1.100     1.100 peak  5762 weight  0.11000E+01 volume  0.82932E+03 ppm1     2.387 ppm2     3.591
ASSI ( 5772)
  (( segid "BrD " and resid 57   and name HD2 ))
  (( segid "BrD " and resid 57   and name HE1 ))
    2.100     1.100     1.100 peak  5772 weight  0.11000E+01 volume  0.96087E+03 ppm1     2.289 ppm2     3.591
ASSI ( 5792)
  (( segid "BrD " and resid 12   and name HA  ))
  (( segid "BrD " and resid 12   and name HB2 ))
    2.700     1.800     1.800 peak  5792 weight  0.11000E+01 volume  0.22035E+03 ppm1     5.297 ppm2     3.338
ASSI ( 5812)
  (( segid "BrD " and resid 57   and name HG1 ))
  (( segid "BrD " and resid 57   and name HE1 ))
    2.600     1.700     1.700 peak  5812 weight  0.11000E+01 volume  0.23002E+03 ppm1     2.099 ppm2     3.590
ASSI ( 5822)
  (( segid "BrD " and resid 26   and name HA  ))
  (( segid "BrD " and resid 26   and name HB1 ))
    2.100     1.100     1.100 peak  5822 weight  0.11000E+01 volume  0.10358E+04 ppm1     4.509 ppm2     2.482
ASSI ( 5832)
  (( segid "BrD " and resid 26   and name HA  ))
  (( segid "BrD " and resid 26   and name HD1 ))
    2.700     1.800     1.800 peak  5832 weight  0.11000E+01 volume  0.18918E+03 ppm1     4.509 ppm2     2.109
ASSI ( 5842)
  (( segid "BrD " and resid 26   and name HA  ))
  (( segid "BrD " and resid 26   and name HG1 ))
    3.200     2.600     2.300 peak  5842 weight  0.11000E+01 volume  0.75991E+02 ppm1     4.509 ppm2     1.629
ASSI ( 5852)
  (( segid "BrD " and resid 10   and name HA  ))
  (( segid "BrD " and resid 10   and name HB2 ))
    2.800     2.000     2.000 peak  5852 weight  0.11000E+01 volume  0.18381E+03 ppm1     5.478 ppm2     3.300
ASSI ( 5862)
  (( segid "BrD " and resid 56   and name HA  ))
  (( segid "BrD " and resid 56   and name HB2 ))
    2.800     2.000     2.000 peak  5862 weight  0.11000E+01 volume  0.18369E+03 ppm1     4.607 ppm2     2.003
ASSI ( 5872)
  (  segid "BrD " and resid 56   and name HD2%)
  (( segid "BrD " and resid 56   and name HB2 ))
    2.600     1.700     1.700 peak  5872 weight  0.11000E+01 volume  0.24752E+03 ppm1     1.254 ppm2     2.004
ASSI ( 5882)
  (  segid "BrD " and resid 69   and name HG1%)
  (( segid "BrD " and resid 69   and name HB  ))
    2.100     1.100     1.100 peak  5882 weight  0.11000E+01 volume  0.96122E+03 ppm1     1.548 ppm2     2.922
ASSI ( 5892)
  (  segid "BrD " and resid 69   and name HG2%)
  (( segid "BrD " and resid 69   and name HB  ))
    2.100     1.100     1.100 peak  5892 weight  0.11000E+01 volume  0.91489E+03 ppm1     1.424 ppm2     2.919
ASSI ( 5902)
  (  segid "BrD " and resid 69   and name HG2%)
  (( segid "BrD " and resid 69   and name HA  ))
    2.600     1.700     1.700 peak  5902 weight  0.11000E+01 volume  0.26227E+03 ppm1     1.425 ppm2     4.696
ASSI ( 5912)
  (  segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 78   and name HA  ))
    2.800     2.000     2.000 peak  5912 weight  0.11000E+01 volume  0.18293E+03 ppm1     0.662 ppm2     3.999
ASSI ( 5922)
  (  segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 78   and name HB2 ))
    2.600     1.700     1.700 peak  5922 weight  0.11000E+01 volume  0.24706E+03 ppm1     0.662 ppm2     1.039
ASSI ( 5932)
  (  segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 78   and name HG  ))
    2.300     1.300     1.300 peak  5932 weight  0.11000E+01 volume  0.60283E+03 ppm1     0.662 ppm2     1.270
ASSI ( 5962)
  (( segid "BrD " and resid 18   and name HA  ))
  (  segid "BrD " and resid 18   and name HD1%)
    2.600     1.700     1.700 peak  5962 weight  0.11000E+01 volume  0.27810E+03 ppm1     3.867 ppm2     1.079
ASSI ( 5982)
  (  segid "BrD " and resid 18   and name HD1%)
  (( segid "BrD " and resid 18   and name HG  ))
    2.700     1.800     1.800 peak  5982 weight  0.11000E+01 volume  0.22916E+03 ppm1     1.057 ppm2     2.278
ASSI ( 5992)
  (  segid "BrD " and resid 18   and name HD2%)
  (( segid "BrD " and resid 18   and name HB1 ))
    2.600     1.700     1.700 peak  5992 weight  0.11000E+01 volume  0.25721E+03 ppm1     0.416 ppm2     2.137
ASSI ( 6002)
  (( segid "BrD " and resid 102  and name HG  ))
  (  segid "BrD " and resid 102  and name HD1%)
    2.300     1.300     1.300 peak  6002 weight  0.11000E+01 volume  0.47853E+03 ppm1     2.141 ppm2     1.324
ASSI ( 6012)
  (( segid "BrD " and resid 73   and name HB1 ))
  (  segid "BrD " and resid 73   and name HD2%)
    2.300     1.300     1.300 peak  6012 weight  0.11000E+01 volume  0.54334E+03 ppm1     2.583 ppm2     1.483
ASSI ( 6052)
  (( segid "BrD " and resid 73   and name HA  ))
  (( segid "BrD " and resid 73   and name HB1 ))
    2.400     1.400     1.400 peak  6052 weight  0.11000E+01 volume  0.44904E+03 ppm1     4.809 ppm2     2.894
ASSI ( 6072)
  (  segid "BrD " and resid 73   and name HD1%)
  (( segid "BrD " and resid 73   and name HA  ))
    2.500     1.600     1.600 peak  6072 weight  0.11000E+01 volume  0.30560E+03 ppm1     1.549 ppm2     4.825
ASSI ( 6112)
  (( segid "BrD " and resid 56   and name HB1 ))
  (  segid "BrD " and resid 56   and name HD1%)
    2.700     1.800     1.800 peak  6112 weight  0.11000E+01 volume  0.20480E+03 ppm1     2.685 ppm2     1.538
ASSI ( 6122)
  (( segid "BrD " and resid 56   and name HB2 ))
  (  segid "BrD " and resid 56   and name HD1%)
    2.900     2.100     2.100 peak  6122 weight  0.11000E+01 volume  0.13067E+03 ppm1     1.994 ppm2     1.538
ASSI ( 6162)
  (( segid "BrD " and resid 56   and name HG  ))
  (  segid "BrD " and resid 56   and name HD1%)
    2.300     1.300     1.300 peak  6162 weight  0.11000E+01 volume  0.52968E+03 ppm1     2.339 ppm2     1.539
ASSI ( 6212)
  (( segid "BrD " and resid 22   and name HA  ))
  (  segid "BrD " and resid 22   and name HD1%)
    2.500     1.600     1.600 peak  6212 weight  0.11000E+01 volume  0.33531E+03 ppm1     4.706 ppm2     1.648
ASSI ( 6232)
  (  segid "BrD " and resid 22   and name HD1%)
  (( segid "BrD " and resid 22   and name HB1 ))
    2.400     1.400     1.400 peak  6232 weight  0.11000E+01 volume  0.37274E+03 ppm1     1.648 ppm2     2.702
ASSI ( 6242)
  (  segid "BrD " and resid 22   and name HD1%)
  (( segid "BrD " and resid 22   and name HG  ))
    2.200     1.200     1.200 peak  6242 weight  0.11000E+01 volume  0.77165E+03 ppm1     1.648 ppm2     2.361
ASSI ( 6272)
  (  segid "BrD " and resid 63   and name HD2%)
  (( segid "BrD " and resid 63   and name HG  ))
    2.600     1.700     1.700 peak  6272 weight  0.11000E+01 volume  0.24631E+03 ppm1     1.498 ppm2     2.424
ASSI ( 6282)
  (  segid "BrD " and resid 63   and name HD1%)
  (( segid "BrD " and resid 63   and name HG  ))
    2.700     1.800     1.800 peak  6282 weight  0.11000E+01 volume  0.21603E+03 ppm1     1.649 ppm2     2.424
ASSI ( 6322)
  (( segid "BrD " and resid 66   and name HG2 ))
  (( segid "BrD " and resid 66   and name HD2 ))
    2.500     1.600     1.600 peak  6322 weight  0.11000E+01 volume  0.35570E+03 ppm1     2.140 ppm2     3.637
ASSI ( 6352)
  (( segid "BrD " and resid 66   and name HD2 ))
  (( segid "BrD " and resid 66   and name HA  ))
    2.500     1.600     1.600 peak  6352 weight  0.11000E+01 volume  0.30900E+03 ppm1     3.631 ppm2     4.996
ASSI ( 6392)
  (( segid "BrD " and resid 100  and name HB1 ))
  (( segid "BrD " and resid 100  and name HA  ))
    2.100     1.100     1.100 peak  6392 weight  0.11000E+01 volume  0.94220E+03 ppm1     3.455 ppm2     4.949
ASSI ( 6412)
  (( segid "BrD " and resid 114  and name HA1 ))
  (( segid "BrD " and resid 114  and name HA2 ))
    2.100     1.100     1.100 peak  6412 weight  0.11000E+01 volume  0.97579E+03 ppm1     4.600 ppm2     4.522
ASSI ( 6432)
  (( segid "BrD " and resid 85   and name HA  ))
  (( segid "BrD " and resid 85   and name HB1 ))
    2.700     1.800     1.800 peak  6432 weight  0.11000E+01 volume  0.21987E+03 ppm1     5.001 ppm2     3.906
ASSI ( 6442)
  (( segid "BrD " and resid 85   and name HA  ))
  (( segid "BrD " and resid 85   and name HB2 ))
    2.800     2.000     2.000 peak  6442 weight  0.11000E+01 volume  0.16015E+03 ppm1     5.000 ppm2     3.621
ASSI ( 6492)
  (( segid "BrD " and resid 98   and name HA  ))
  (( segid "BrD " and resid 98   and name HB1 ))
    2.800     2.000     2.000 peak  6492 weight  0.11000E+01 volume  0.16821E+03 ppm1     4.804 ppm2     4.014
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ASSI ( 6502)
  (( segid "BrD " and resid 98   and name HA  ))
  (( segid "BrD " and resid 98   and name HB2 ))
    2.700     1.800     1.800 peak  6502 weight  0.11000E+01 volume  0.19206E+03 ppm1      4.804 ppm2      3.660
ASSI ( 6512)
  (( segid "BrD " and resid 32   and name HA  ))
  (( segid "BrD " and resid 32   and name HB2 ))
    2.700     1.800     1.800 peak  6512 weight  0.11000E+01 volume  0.22946E+03 ppm1      4.953 ppm2      3.965
ASSI ( 6522)
  (( segid "BrD " and resid 32   and name HA  ))
  (( segid "BrD " and resid 32   and name HB1 ))
    2.700     1.800     1.800 peak  6522 weight  0.11000E+01 volume  0.20617E+03 ppm1      4.954 ppm2      4.206
ASSI ( 6552)
  (( segid "BrD " and resid 11   and name HA  ))
  (( segid "BrD " and resid 11   and name HG1 ))
    2.600     1.700     1.700 peak  6552 weight  0.11000E+01 volume  0.23807E+03 ppm1      4.951 ppm2      2.635
ASSI ( 6562)
  (( segid "BrD " and resid 53   and name HG1 ))
  (( segid "BrD " and resid 53   and name HA  ))
    2.700     1.800     1.800 peak  6562 weight  0.11000E+01 volume  0.20893E+03 ppm1      2.784 ppm2      4.687
ASSI ( 6572)
  (( segid "BrD " and resid 31   and name HA  ))
  (  segid "BrD " and resid 102  and name HD1%)
    2.500     1.600     1.600 peak  6572 weight  0.11000E+01 volume  0.36090E+03 ppm1      5.000 ppm2      1.323
ASSI ( 6612)
  (  segid "BrD " and resid 31   and name HB% )
  (  segid "BrD " and resid 102  and name HD1%)
    2.500     1.600     1.600 peak  6612 weight  0.11000E+01 volume  0.31261E+03 ppm1      2.289 ppm2      1.320
ASSI ( 6642)
  (( segid "BrD " and resid 43   and name HA  ))
  (( segid "BrD " and resid 44   and name HD2 ))
    2.400     1.400     1.400 peak  6642 weight  0.11000E+01 volume  0.39697E+03 ppm1      5.547 ppm2      4.127
ASSI ( 6662)
  (  segid "BrD " and resid 43   and name HB% )
  (( segid "BrD " and resid 44   and name HD2 ))
    2.700     1.800     1.800 peak  6662 weight  0.11000E+01 volume  0.20471E+03 ppm1      1.700 ppm2      4.135
ASSI ( 6672)
  (  segid "BrD " and resid 43   and name HB% )
  (( segid "BrD " and resid 46   and name HB1 ))
    2.600     1.700     1.700 peak  6672 weight  0.11000E+01 volume  0.27100E+03 ppm1      1.697 ppm2      3.295
ASSI ( 6682)
  (  segid "BrD " and resid 43   and name HB% )
  (( segid "BrD " and resid 46   and name HB2 ))
    2.700     1.800     1.800 peak  6682 weight  0.11000E+01 volume  0.19809E+03 ppm1      1.697 ppm2      3.100
ASSI ( 6732)
  (( segid "BrD " and resid 76   and name HA  ))
  (( segid "BrD " and resid 79   and name HB1 ))
    2.800     2.000     2.000 peak  6732 weight  0.11000E+01 volume  0.16513E+03 ppm1      4.658 ppm2      2.774
ASSI ( 6872)
  (  segid "BrD " and resid 113  and name HB% )
  (  segid "BrD " and resid 17   and name HG2%)
    2.500     1.600     1.600 peak  6872 weight  0.11000E+01 volume  0.31889E+03 ppm1      1.994 ppm2      1.750
ASSI ( 6882)
  (( segid "BrD " and resid 79   and name HA  ))
  (( segid "BrD " and resid 79   and name HB1 ))
    2.700     1.800     1.800 peak  6882 weight  0.11000E+01 volume  0.19089E+03 ppm1      4.409 ppm2      2.781
ASSI ( 6892)
  (( segid "BrD " and resid 79   and name HA  ))
  (( segid "BrD " and resid 79   and name HB2 ))
    2.200     1.200     1.200 peak  6892 weight  0.11000E+01 volume  0.79324E+03 ppm1      4.409 ppm2      2.678
ASSI ( 6912)
  (  segid "BrD " and resid 43   and name HB% )
  (( segid "BrD " and resid 44   and name HD1 ))
    2.900     2.100     2.100 peak  6912 weight  0.11000E+01 volume  0.13650E+03 ppm1      1.700 ppm2      4.337
ASSI ( 6942)
  (  segid "BrD " and resid 25   and name HG1%)
  (  segid "BrD " and resid 102  and name HD1%)
    2.700     1.800     1.800 peak  6942 weight  0.11000E+01 volume  0.21235E+03 ppm1      1.795 ppm2      1.323
ASSI ( 6962)
  (  segid "BrD " and resid 25   and name HG1%)
  (  segid "BrD " and resid 78   and name HD1%)
    3.000     2.200     2.200 peak  6962 weight  0.11000E+01 volume  0.99662E+02 ppm1      1.798 ppm2      0.774
ASSI ( 6972)
  (  segid "BrD " and resid 25   and name HG1%)
  (  segid "BrD " and resid 78   and name HD2%)
    2.800     2.000     2.000 peak  6972 weight  0.11000E+01 volume  0.15213E+03 ppm1      1.797 ppm2      0.673
ASSI ( 6992)
  (  segid "BrD " and resid 25   and name HG2%)
  (  segid "BrD " and resid 102  and name HD1%)
    2.200     1.200     1.200 peak  6992 weight  0.11000E+01 volume  0.77265E+03 ppm1      1.646 ppm2      1.324
ASSI ( 7002)
  (  segid "BrD " and resid 25   and name HG2%)
  (  segid "BrD " and resid 78   and name HD1%)
    2.800     2.000     2.000 peak  7002 weight  0.11000E+01 volume  0.16697E+03 ppm1      1.646 ppm2      0.775
ASSI ( 7022)
  (( segid "BrD " and resid 38   and name HB  ))
  (( segid "BrD " and resid 38   and name HA  ))
    2.800     2.000     2.000 peak  7022 weight  0.11000E+01 volume  0.17527E+03 ppm1      1.751 ppm2      4.170
ASSI ( 7032)
  (  segid "BrD " and resid 38   and name HG2%)
  (  segid "BrD " and resid 43   and name HB% )
    2.200     1.200     1.200 peak  7032 weight  0.11000E+01 volume  0.74974E+03 ppm1      0.608 ppm2      1.715
ASSI ( 7092)
  (( segid "BrD " and resid 81   and name HA  ))
  (( segid "BrD " and resid 81   and name HB  ))
    2.800     2.000     2.000 peak  7092 weight  0.11000E+01 volume  0.15196E+03 ppm1      3.718 ppm2      2.037
ASSI ( 7102)
  (( segid "BrD " and resid 81   and name HB  ))
  (( segid "BrD " and resid 78   and name HA  ))
    3.100     2.400     2.400 peak  7102 weight  0.11000E+01 volume  0.98817E+02 ppm1      2.042 ppm2      4.000
ASSI ( 7122)
  (  segid "BrD " and resid 81   and name HG1%)
  (( segid "BrD " and resid 78   and name HA  ))
    2.600     1.700     1.700 peak  7122 weight  0.11000E+01 volume  0.25254E+03 ppm1      1.059 ppm2      3.999
ASSI ( 7172)
  (  segid "BrD " and resid 81   and name HG2%)
  (( segid "BrD " and resid 34   and name HB1 ))
    2.600     1.700     1.700 peak  7172 weight  0.11000E+01 volume  0.27152E+03 ppm1      0.755 ppm2      4.106
ASSI ( 7192)
  (( segid "BrD " and resid 17   and name HA  ))
  (( segid "BrD " and resid 20   and name HB1 ))
    3.200     2.600     2.300 peak  7192 weight  0.11000E+01 volume  0.76028E+02 ppm1      4.562 ppm2      4.671
ASSI ( 7252)
  (  segid "BrD " and resid 17   and name HG2%)
  (  segid "BrD " and resid 102  and name HD2%)
    5.500     5.500     0.000 peak  7252 weight  0.11000E+01 volume  0.56051E+00 ppm1      1.746 ppm2      1.320
ASSI ( 7272)
  (  segid "BrD " and resid 17   and name HG2%)
  (  segid "BrD " and resid 18   and name HD2%)
    2.800     2.000     2.000 peak  7272 weight  0.11000E+01 volume  0.14970E+03 ppm1      1.747 ppm2      0.409
ASSI ( 7352)
  (  segid "BrD " and resid 58   and name HG2%)
  (  segid "BrD " and resid 54   and name HE% )
    2.400     1.400     1.400 peak  7352 weight  0.11000E+01 volume  0.41514E+03 ppm1      1.649 ppm2      2.863
ASSI ( 7482)
  (( segid "BrD " and resid 32   and name HA  ))
  (( segid "BrD " and resid 35   and name HG1 ))
    2.900     2.100     2.100 peak  7482 weight  0.11000E+01 volume  0.12205E+03 ppm1      4.953 ppm2      3.451
ASSI ( 7492)
  (( segid "BrD " and resid 32   and name HA  ))
  (( segid "BrD " and resid 33   and name HD1 ))
    2.900     2.100     2.100 peak  7492 weight  0.11000E+01 volume  0.14430E+03 ppm1      4.952 ppm2      2.776
ASSI ( 7502)
  (( segid "BrD " and resid 62   and name HA  ))
  (( segid "BrD " and resid 62   and name HB1 ))
    2.700     1.800     1.800 peak  7502 weight  0.11000E+01 volume  0.21435E+03 ppm1      4.457 ppm2      2.657
ASSI ( 7522)
  (( segid "BrD " and resid 62   and name HA  ))
  (( segid "BrD " and resid 62   and name HG2 ))
    2.800     2.000     2.000 peak  7522 weight  0.11000E+01 volume  0.15009E+03 ppm1      4.457 ppm2      1.478
ASSI ( 7532)
  (( segid "BrD " and resid 62   and name HA  ))
  (( segid "BrD " and resid 62   and name HB2 ))
    3.000     2.200     2.200 peak  7532 weight  0.11000E+01 volume  0.10361E+03 ppm1      4.457 ppm2      1.681
ASSI ( 7652)
  (( segid "BrD " and resid 74   and name HA  ))
  (  segid "BrD " and resid 59   and name HE% )
    3.100     2.400     2.400 peak  7652 weight  0.11000E+01 volume  0.93787E+02 ppm1      4.361 ppm2      1.879
ASSI ( 7662)
  (( segid "BrD " and resid 74   and name HB1 ))
  (( segid "BrD " and resid 71   and name HA  ))
    3.100     2.400     2.400 peak  7662 weight  0.11000E+01 volume  0.98803E+02 ppm1      3.576 ppm2      4.627
ASSI ( 7722)
  (( segid "BrD " and resid 105  and name HA  ))
  (( segid "BrD " and resid 108  and name HB1 ))
    3.100     2.400     2.400 peak  7722 weight  0.11000E+01 volume  0.93160E+02 ppm1      4.902 ppm2      4.582
ASSI ( 7752)
  (( segid "BrD " and resid 107  and name HA  ))
  (( segid "BrD " and resid 110  and name HB  ))
    2.800     2.000     2.000 peak  7752 weight  0.11000E+01 volume  0.15544E+03 ppm1      4.410 ppm2      2.360
ASSI ( 7762)
  (( segid "BrD " and resid 96   and name HA  ))
  (  segid "BrD " and resid 99   and name HB% )
    3.400     2.900     3.100 peak  7762 weight  0.11000E+01 volume  0.54211E+02 ppm1      4.409 ppm2      2.206
ASSI ( 7772)
  (( segid "BrD " and resid 107  and name HA  ))
  (( segid "BrD " and resid 110  and name HG11))
    3.100     2.400     2.400 peak  7772 weight  0.11000E+01 volume  0.86608E+02 ppm1      4.408 ppm2      1.715
ASSI ( 7782)
  (( segid "BrD " and resid 107  and name HA  ))
  (( segid "BrD " and resid 110  and name HG12))
    2.900     2.100     2.100 peak  7782 weight  0.11000E+01 volume  0.14800E+03 ppm1      4.408 ppm2      1.661
ASSI ( 7792)
  (( segid "BrD " and resid 107  and name HA  ))
  (  segid "BrD " and resid 110  and name HG2%)
    3.100     2.400     2.400 peak  7792 weight  0.11000E+01 volume  0.86153E+02 ppm1      4.408 ppm2      1.261
ASSI ( 7802)
  (( segid "BrD " and resid 107  and name HA  ))
  (  segid "BrD " and resid 110  and name HD1%)
    3.000     2.200     2.200 peak  7802 weight  0.11000E+01 volume  0.11960E+03 ppm1      4.408 ppm2      1.141
ASSI ( 7872)
  (( segid "BrD " and resid 89   and name HA  ))
  (( segid "BrD " and resid 91   and name HD2 ))
    2.700     1.800     1.800 peak  7872 weight  0.11000E+01 volume  0.22343E+03 ppm1      5.641 ppm2      4.407
ASSI ( 7892)
  (( segid "BrD " and resid 100  and name HA  ))
  (( segid "BrD " and resid 103  and name HB2 ))
    2.900     2.100     2.100 peak  7892 weight  0.11000E+01 volume  0.12930E+03 ppm1      4.952 ppm2      1.897
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ASSI [ 7922]
  (( segid "BrD " and resid 100  and name HB1 ))
  (( segid "BrD " and resid 97   and name HA  ))
     2.600     1.700     1.700 peak  7922 weight  0.11000E+01 volume  0.24354E+03 ppm1     3.455 ppm2     4.798
ASSI [ 7932]
  (( segid "BrD " and resid 100  and name HB2 ))
  (( segid "BrD " and resid 97   and name HA  ))
     2.600     1.700     1.700 peak  7932 weight  0.11000E+01 volume  0.23409E+03 ppm1     3.424 ppm2     4.799
ASSI [ 7962]
  (( segid "BrD " and resid 12   and name HA  ))
  (( segid "BrD " and resid 15   and name HB2 ))
     2.900     2.100     2.100 peak  7962 weight  0.11000E+01 volume  0.12451E+03 ppm1     5.298 ppm2     3.646
ASSI [ 7972]
  (( segid "BrD " and resid 12   and name HA  ))
  (( segid "BrD " and resid 15   and name HB1 ))
     3.100     2.400     2.400 peak  7972 weight  0.11000E+01 volume  0.81954E+02 ppm1     5.297 ppm2     3.812
ASSI [ 8032]
  (( segid "BrD " and resid 77   and name HA  ))
  (( segid "BrD " and resid 80   and name HG1 ))
     3.000     2.200     2.200 peak  8032 weight  0.11000E+01 volume  0.10885E+03 ppm1     4.952 ppm2     2.347
ASSI [ 8062]
  (( segid "BrD " and resid 85   and name HB2 ))
  (( segid "BrD " and resid 82   and name HA  ))
     3.000     2.200     2.200 peak  8062 weight  0.11000E+01 volume  0.10120E+03 ppm1     3.621 ppm2     4.753
ASSI [ 8072]
  (( segid "BrD " and resid 98   and name HB2 ))
  (( segid "BrD " and resid 95   and name HA  ))
     3.100     2.400     2.400 peak  8072 weight  0.11000E+01 volume  0.94016E+02 ppm1     3.667 ppm2     4.447
ASSI [ 8102]
  (( segid "BrD " and resid 63   and name HB1 ))
  (( segid "BrD " and resid 60   and name HA  ))
     2.600     1.700     1.700 peak  8102 weight  0.11000E+01 volume  0.27762E+03 ppm1     2.883 ppm2     4.808
ASSI [ 8112]
  (( segid "BrD " and resid 63   and name HB2 ))
  (( segid "BrD " and resid 60   and name HA  ))
     2.700     1.800     1.800 peak  8112 weight  0.11000E+01 volume  0.20887E+03 ppm1     2.538 ppm2     4.809
ASSI [ 8142]
  (  segid "BrD " and resid 63   and name HD1%)
  (( segid "BrD " and resid 18   and name HB2 ))
     2.800     2.000     2.000 peak  8142 weight  0.11000E+01 volume  0.16157E+03 ppm1     1.649 ppm2     0.919
ASSI [ 8152]
  (  segid "BrD " and resid 63   and name HD1%)
  (  segid "BrD " and resid 18   and name HD1%)
     2.700     1.800     1.800 peak  8152 weight  0.11000E+01 volume  0.20633E+03 ppm1     1.646 ppm2     1.085
ASSI [ 8162]
  (  segid "BrD " and resid 63   and name HD1%)
  (( segid "BrD " and resid 18   and name HB1 ))
     2.400     1.400     1.400 peak  8162 weight  0.11000E+01 volume  0.38153E+03 ppm1     1.649 ppm2     2.139
ASSI [ 8172]
  (  segid "BrD " and resid 63   and name HD2%)
  (( segid "BrD " and resid 19   and name HA  ))
     2.400     1.400     1.400 peak  8172 weight  0.11000E+01 volume  0.45741E+03 ppm1     1.501 ppm2     4.295
ASSI [ 8182]
  (( segid "BrD " and resid 14   and name HB2 ))
  (( segid "BrD " and resid 14   and name HG  ))
     3.100     2.400     2.400 peak  8182 weight  0.11000E+01 volume  0.92156E+02 ppm1     2.145 ppm2     2.059
ASSI [ 8192]
  (( segid "BrD " and resid 14   and name HB1 ))
  (( segid "BrD " and resid 14   and name HG  ))
     2.600     1.700     1.700 peak  8192 weight  0.11000E+01 volume  0.23309E+03 ppm1     2.444 ppm2     2.059
ASSI [ 8222]
  (  segid "BrD " and resid 14   and name HD2%)
  (  segid "BrD " and resid 18   and name HD2%)
     2.500     1.600     1.600 peak  8222 weight  0.11000E+01 volume  0.31711E+03 ppm1     1.401 ppm2     0.409
ASSI [ 8232]
  (  segid "BrD " and resid 14   and name HD2%)
  (  segid "BrD " and resid 18   and name HD1%)
     2.400     1.400     1.400 peak  8232 weight  0.11000E+01 volume  0.46026E+03 ppm1     1.401 ppm2     1.085
ASSI [ 8302]
  (( segid "BrD " and resid 18   and name HA  ))
  (( segid "BrD " and resid 15   and name HB2 ))
     2.700     1.800     1.800 peak  8302 weight  0.11000E+01 volume  0.20320E+03 ppm1     3.867 ppm2     0.920
ASSI [ 8392]
  (  segid "BrD " and resid 18   and name HD1%)
  (( segid "BrD " and resid 18   and name HB2 ))
     2.400     1.400     1.400 peak  8392 weight  0.11000E+01 volume  0.39910E+03 ppm1     1.057 ppm2     0.925
ASSI [ 8402]
  (  segid "BrD " and resid 18   and name HD1%)
  (( segid "BrD " and resid 74   and name HB1 ))
     3.000     2.200     2.200 peak  8402 weight  0.11000E+01 volume  0.10291E+03 ppm1     1.056 ppm2     3.563
ASSI [ 8412]
  (  segid "BrD " and resid 18   and name HD1%)
  (( segid "BrD " and resid 74   and name HB2 ))
     2.900     2.100     2.100 peak  8412 weight  0.11000E+01 volume  0.13686E+03 ppm1     1.057 ppm2     2.998
ASSI [ 8442]
  (  segid "BrD " and resid 18   and name HD2%)
  (  segid "BrD " and resid 14   and name HD1%)
     2.900     2.100     2.100 peak  8442 weight  0.11000E+01 volume  0.12935E+03 ppm1     0.412 ppm2     1.417
ASSI [ 8452]
  (  segid "BrD " and resid 18   and name HD2%)
  (( segid "BrD " and resid 18   and name HB2 ))
     2.800     2.000     2.000 peak  8452 weight  0.11000E+01 volume  0.15454E+03 ppm1     0.415 ppm2     0.917
ASSI [ 8462]
  (  segid "BrD " and resid 18   and name HD2%)
  (  segid "BrD " and resid 102  and name HD2%)
     5.500     5.500     0.000 peak  8462 weight  0.11000E+01 volume  0.22428E+01 ppm1     0.416 ppm2     1.320
ASSI [ 8552]
  (( segid "BrD " and resid 22   and name HB1 ))
  (( segid "BrD " and resid 19   and name HA  ))
     2.600     1.700     1.700 peak  8552 weight  0.11000E+01 volume  0.27759E+03 ppm1     2.682 ppm2     4.295
ASSI [ 8562]
  (( segid "BrD " and resid 22   and name HB2 ))
  (  segid "BrD " and resid 22   and name HD1%)
     2.500     1.600     1.600 peak  8562 weight  0.11000E+01 volume  0.30282E+03 ppm1     2.286 ppm2     1.671
ASSI [ 8602]
  (( segid "BrD " and resid 22   and name HA  ))
  (( segid "BrD " and resid 25   and name HB  ))
     2.600     1.700     1.700 peak  8602 weight  0.11000E+01 volume  0.25684E+03 ppm1     4.706 ppm2     2.980
ASSI [ 8652]
  (  segid "BrD " and resid 56   and name HD1%)
  (( segid "BrD " and resid 56   and name HA  ))
     2.500     1.600     1.600 peak  8652 weight  0.11000E+01 volume  0.34689E+03 ppm1     1.544 ppm2     4.638
ASSI [ 8672]
  (  segid "BrD " and resid 56   and name HD2%)
  (  segid "BrD " and resid 78   and name HD2%)
     2.900     2.100     2.100 peak  8672 weight  0.11000E+01 volume  0.14779E+03 ppm1     1.253 ppm2     0.674
ASSI [ 8682]
  (  segid "BrD " and resid 56   and name HD2%)
  (  segid "BrD " and resid 78   and name HD1%)
     2.300     1.300     1.300 peak  8682 weight  0.11000E+01 volume  0.48347E+03 ppm1     1.254 ppm2     0.767
ASSI [ 8722]
  (( segid "BrD " and resid 73   and name HA  ))
  (  segid "BrD " and resid 76   and name HB% )
     2.700     1.800     1.800 peak  8722 weight  0.11000E+01 volume  0.22156E+03 ppm1     4.805 ppm2     2.101
ASSI [ 8742]
  (  segid "BrD " and resid 73   and name HD1%)
  (( segid "BrD " and resid 73   and name HB1 ))
     2.400     1.400     1.400 peak  8742 weight  0.11000E+01 volume  0.42630E+03 ppm1     1.549 ppm2     2.594
ASSI [ 8752]
  (( segid "BrD " and resid 78   and name HA  ))
  (  segid "BrD " and resid 59   and name HE% )
     3.300     2.700     2.300 peak  8752 weight  0.11000E+01 volume  0.67002E+02 ppm1     3.967 ppm2     1.876
ASSI [ 8782]
  (( segid "BrD " and resid 78   and name HB1 ))
  (  segid "BrD " and resid 59   and name HE% )
     3.200     2.600     2.300 peak  8782 weight  0.11000E+01 volume  0.75592E+02 ppm1     1.307 ppm2     1.876
ASSI [ 8792]
  (( segid "BrD " and resid 78   and name HB2 ))
  (  segid "BrD " and resid 59   and name HE% )
     2.900     2.100     2.100 peak  8792 weight  0.11000E+01 volume  0.13244E+03 ppm1     1.054 ppm2     1.876
ASSI [ 8802]
  (( segid "BrD " and resid 78   and name HB1 ))
  (( segid "BrD " and resid 75   and name HA  ))
     3.100     2.400     2.400 peak  8802 weight  0.11000E+01 volume  0.93675E+02 ppm1     1.305 ppm2     4.520
ASSI [ 8812]
  (( segid "BrD " and resid 78   and name HG  ))
  (  segid "BrD " and resid 59   and name HE% )
     3.200     2.600     2.300 peak  8812 weight  0.11000E+01 volume  0.81269E+02 ppm1     1.254 ppm2     1.878
ASSI [ 8822]
  (  segid "BrD " and resid 76   and name HD1%)
  (  segid "BrD " and resid 81   and name HG1%)
     2.600     1.700     1.700 peak  8822 weight  0.11000E+01 volume  0.25375E+03 ppm1     0.761 ppm2     1.078
ASSI [ 8852]
  (  segid "BrD " and resid 78   and name HD1%)
  (  segid "BrD " and resid 59   and name HE% )
     2.900     2.100     2.100 peak  8852 weight  0.11000E+01 volume  0.13937E+03 ppm1     0.761 ppm2     1.875
ASSI [ 8872]
  (  segid "BrD " and resid 78   and name HD2%)
  (  segid "BrD " and resid 25   and name HG2%)
     2.600     1.700     1.700 peak  8872 weight  0.11000E+01 volume  0.25847E+03 ppm1     0.662 ppm2     1.637
ASSI [ 8892]
  (  segid "BrD " and resid 78   and name HD2%)
  (  segid "BrD " and resid 81   and name HG1%)
     2.800     2.000     2.000 peak  8892 weight  0.11000E+01 volume  0.17974E+03 ppm1     0.662 ppm2     1.078
ASSI [ 8912]
  (  segid "BrD " and resid 78   and name HD2%)
  (  segid "BrD " and resid 59   and name HE% )
     2.600     1.700     1.700 peak  8912 weight  0.11000E+01 volume  0.24075E+03 ppm1     0.662 ppm2     1.875
ASSI [ 8922]
  (( segid "BrD " and resid 102  and name HA  ))
  (( segid "BrD " and resid 105  and name HB1 ))
     2.800     2.000     2.000 peak  8922 weight  0.11000E+01 volume  0.18319E+03 ppm1     4.263 ppm2     3.743
ASSI [ 8932]
  (( segid "BrD " and resid 102  and name HA  ))
  (( segid "BrD " and resid 105  and name HB2 ))
     2.700     1.800     1.800 peak  8932 weight  0.11000E+01 volume  0.21483E+03 ppm1     4.263 ppm2     3.674
ASSI [ 8952]
  (( segid "BrD " and resid 102  and name HB1 ))
  (( segid "BrD " and resid 99   and name HA  ))
     2.900     2.100     2.100 peak  8952 weight  0.11000E+01 volume  0.14144E+03 ppm1     1.993 ppm2     4.442
ASSI [ 8972]
  (  segid "BrD " and resid 102  and name HD1%)
  (( segid "BrD " and resid 25   and name HA  ))
     2.700     1.800     1.800 peak  8972 weight  0.11000E+01 volume  0.20447E+03 ppm1     1.303 ppm2     4.434
ASSI [ 8982]
  (  segid "BrD " and resid 102  and name HD1%)
  (( segid "BrD " and resid 105  and name HB1 ))
     3.000     3.200     3.200 peak  8982 weight  0.11000E+01 volume  0.11841E+03 ppm1     1.303 ppm2     3.760
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ASSI ( 8992)
  (  segid "BrD " and resid 102  and name HD1%)
  (( segid "BrD " and resid 105  and name HB2 ))
     2.800      2.000      2.000 peak  8992 weight  0.11000E+01 volume  0.16956E+03 ppm1      1.303 ppm2      3.689
ASSI ( 9002)
  (  segid "BrD " and resid 102  and name HD1%)
  (( segid "BrD " and resid 28   and name HB1 ))
     2.600      1.700      1.700 peak  9002 weight  0.11000E+01 volume  0.27744E+03 ppm1      1.303 ppm2      3.603
ASSI ( 9012)
  (  segid "BrD " and resid 102  and name HD1%)
  (( segid "BrD " and resid 28   and name HB2 ))
     2.800      2.000      2.000 peak  9012 weight  0.11000E+01 volume  0.15194E+03 ppm1      1.303 ppm2      3.402
ASSI ( 9062)
  (( segid "BrD " and resid 115  and name HB1 ))
  (  segid "BrD " and resid 115  and name HD1%)
     2.300      1.300      1.300 peak  9062 weight  0.11000E+01 volume  0.58334E+03 ppm1      2.190 ppm2      1.348
ASSI ( 9082)
  (( segid "BrD " and resid 21   and name HA  ))
  (( segid "BrD " and resid 24   and name HB1 ))
     3.000      2.200      2.200 peak  9082 weight  0.11000E+01 volume  0.11815E+03 ppm1      4.360 ppm2      3.074
ASSI ( 9092)
  (( segid "BrD " and resid 21   and name HB  ))
  (( segid "BrD " and resid 18   and name HA  ))
     2.400      2.000      2.000 peak  9092 weight  0.11000E+01 volume  0.16218E+03 ppm1      2.488 ppm2      3.864
ASSI ( 9182)
  (  segid "BrD " and resid 21   and name HD1%)
  (  segid "BrD " and resid 18   and name HD2%)
     2.900      2.100      2.100 peak  9182 weight  0.11000E+01 volume  0.13133E+03 ppm1      1.203 ppm2      0.410
ASSI ( 9222)
  (  segid "BrD " and resid 21   and name HD1%)
  (( segid "BrD " and resid 18   and name HA  ))
     2.900      2.100      2.100 peak  9222 weight  0.11000E+01 volume  0.13713E+03 ppm1      1.205 ppm2      3.883
ASSI ( 9242)
  (( segid "BrD " and resid 50   and name HG11))
  (( segid "BrD " and resid 50   and name HG12))
     2.500      1.600      1.600 peak  9242 weight  0.11000E+01 volume  0.31566E+03 ppm1      1.397 ppm2      0.834
ASSI ( 9292)
  (  segid "BrD " and resid 50   and name HG2%)
  (( segid "BrD " and resid 53   and name HB1 ))
     2.700      1.800      1.800 peak  9292 weight  0.11000E+01 volume  0.22449E+03 ppm1      1.006 ppm2      2.820
ASSI ( 9302)
  (  segid "BrD " and resid 50   and name HG2%)
  (( segid "BrD " and resid 53   and name HG2 ))
     3.100      2.400      2.400 peak  9302 weight  0.11000E+01 volume  0.95431E+02 ppm1      1.006 ppm2      2.500
ASSI ( 9312)
  (  segid "BrD " and resid 50   and name HG2%)
  (( segid "BrD " and resid 84   and name HB2 ))
     2.800      2.000      2.000 peak  9312 weight  0.11000E+01 volume  0.16689E+03 ppm1      1.004 ppm2      3.271
ASSI ( 9322)
  (  segid "BrD " and resid 50   and name HG2%)
  (( segid "BrD " and resid 51   and name HA  ))
     2.500      1.600      1.600 peak  9322 weight  0.11000E+01 volume  0.33859E+03 ppm1      1.008 ppm2      4.690
ASSI ( 9332)
  (( segid "BrD " and resid 101  and name HA  ))
  (( segid "BrD " and resid 104  and name HD1 ))
     3.000      2.200      2.200 peak  9332 weight  0.11000E+01 volume  0.11803E+03 ppm1      4.265 ppm2      2.302
ASSI ( 9342)
  (( segid "BrD " and resid 101  and name HB  ))
  (( segid "BrD " and resid 98   and name HA  ))
     2.500      1.600      1.600 peak  9342 weight  0.11000E+01 volume  0.31366E+03 ppm1      2.533 ppm2      4.810
ASSI ( 9372)
  (( segid "BrD " and resid 101  and name HG11))
  (( segid "BrD " and resid 101  and name HG12))
     2.300      1.300      1.300 peak  9372 weight  0.11000E+01 volume  0.48997E+03 ppm1      2.444 ppm2      1.807
ASSI ( 9422)
  (  segid "BrD " and resid 101  and name HD1%)
  (( segid "BrD " and resid 98   and name HA  ))
     2.600      1.700      1.700 peak  9422 weight  0.11000E+01 volume  0.26958E+03 ppm1      1.547 ppm2      4.810
ASSI ( 9432)
  (( segid "BrD " and resid 110  and name HA  ))
  (( segid "BrD " and resid 110  and name HG12))
     3.000      2.200      2.200 peak  9432 weight  0.11000E+01 volume  0.11168E+03 ppm1      4.411 ppm2      1.651
ASSI ( 9442)
  (( segid "BrD " and resid 110  and name HA  ))
  (  segid "BrD " and resid 113  and name HB% )
     2.700      1.800      1.800 peak  9442 weight  0.11000E+01 volume  0.20383E+03 ppm1      4.411 ppm2      1.976
ASSI ( 9712)
  (( segid "BrD " and resid 24   and name HA  ))
  (( segid "BrD " and resid 24   and name HB2 ))
     2.500      1.600      1.600 peak  9712 weight  0.11000E+01 volume  0.30771E+03 ppm1      4.784 ppm2      2.989
ASSI ( 9762)
  (( segid "BrD " and resid 23   and name HA  ))
  (( segid "BrD " and resid 23   and name HB2 ))
     2.300      1.300      1.300 peak  9762 weight  0.11000E+01 volume  0.47366E+03 ppm1      4.653 ppm2      2.857
ASSI ( 9772)
  (( segid "BrD " and resid 23   and name HA  ))
  (( segid "BrD " and resid 23   and name HB1 ))
     2.400      1.400      1.400 peak  9772 weight  0.11000E+01 volume  0.38829E+03 ppm1      4.653 ppm2      2.930
ASSI ( 9782)
  (( segid "BrD " and resid 13   and name HB1 ))
  (( segid "BrD " and resid 13   and name HA  ))
     2.900      2.100      2.100 peak  9782 weight  0.11000E+01 volume  0.14088E+03 ppm1      2.733 ppm2      4.775
ASSI ( 9802)
  (( segid "BrD " and resid 103  and name HA  ))
  (( segid "BrD " and resid 103  and name HB2 ))
     2.900      2.100      2.100 peak  9802 weight  0.11000E+01 volume  0.13225E+03 ppm1      3.769 ppm2      1.897
ASSI ( 9812)
  (( segid "BrD " and resid 103  and name HA  ))
  (( segid "BrD " and resid 103  and name HB1 ))
     2.800      2.000      2.000 peak  9812 weight  0.11000E+01 volume  0.16112E+03 ppm1      3.769 ppm2      2.346
ASSI ( 9822)
  (( segid "BrD " and resid 103  and name HA  ))
  (( segid "BrD " and resid 106  and name HB1 ))
     2.800      2.000      2.000 peak  9822 weight  0.11000E+01 volume  0.15761E+03 ppm1      3.769 ppm2      3.917
ASSI ( 9832)
  (( segid "BrD " and resid 103  and name HA  ))
  (( segid "BrD " and resid 106  and name HB2 ))
     2.800      2.000      2.000 peak  9832 weight  0.11000E+01 volume  0.15186E+03 ppm1      3.769 ppm2      3.702
ASSI ( 9862)
  (( segid "BrD " and resid 10   and name HA  ))
  (( segid "BrD " and resid 11   and name HD1 ))
     3.000      2.200      2.200 peak  9862 weight  0.11000E+01 volume  0.11074E+03 ppm1      5.479 ppm2      4.464
ASSI ( 9872)
  (( segid "BrD " and resid 22   and name HB2 ))
  (( segid "BrD " and resid 19   and name HA  ))
     2.800      2.000      2.000 peak  9872 weight  0.11000E+01 volume  0.16684E+03 ppm1      2.286 ppm2      4.297
ASSI ( 9912)
  (( segid "BrD " and resid 36   and name HB1 ))
  (( segid "BrD " and resid 36   and name HA  ))
     2.700      1.800      1.800 peak  9912 weight  0.11000E+01 volume  0.21616E+03 ppm1      2.685 ppm2      5.445
ASSI ( 9922)
  (( segid "BrD " and resid 36   and name HB2 ))
  (( segid "BrD " and resid 36   and name HA  ))
     2.800      2.000      2.000 peak  9922 weight  0.11000E+01 volume  0.17054E+03 ppm1      2.340 ppm2      5.444
ASSI ( 9932)
  (( segid "BrD " and resid 36   and name HB1 ))
  (( segid "BrD " and resid 37   and name HD1 ))
     5.500      5.500      0.000 peak  9932 weight  0.11000E+01 volume  0.21944E+00 ppm1      2.686 ppm2      4.296
ASSI ( 9942)
  (( segid "BrD " and resid 36   and name HB2 ))
  (( segid "BrD " and resid 37   and name HD1 ))
     3.900      3.800      1.600 peak  9942 weight  0.11000E+01 volume  0.23373E+02 ppm1      2.341 ppm2      4.296
ASSI ( 9952)
  (( segid "BrD " and resid 36   and name HG1 ))
  (( segid "BrD " and resid 37   and name HD1 ))
     2.600      1.700      1.700 peak  9952 weight  0.11000E+01 volume  0.23785E+03 ppm1      2.781 ppm2      4.289
ASSI ( 9962)
  (( segid "BrD " and resid 54   and name HB1 ))
  (( segid "BrD " and resid 54   and name HA  ))
     2.900      2.100      2.100 peak  9962 weight  0.11000E+01 volume  0.14616E+03 ppm1      2.585 ppm2      5.542
ASSI ( 9982)
  (( segid "BrD " and resid 54   and name HB2 ))
  (( segid "BrD " and resid 54   and name HG1 ))
     2.900      2.100      2.100 peak  9982 weight  0.11000E+01 volume  0.13342E+03 ppm1      1.947 ppm2      3.304
ASSI (10042)
  (( segid "BrD " and resid 54   and name HA  ))
  (( segid "BrD " and resid 54   and name HG1 ))
     3.400      2.900      2.100 peak 10042 weight  0.11000E+01 volume  0.51922E+02 ppm1      5.541 ppm2      3.304
ASSI (10062)
  (( segid "BrD " and resid 35   and name HA  ))
  (( segid "BrD " and resid 35   and name HB2 ))
     3.000      2.200      2.200 peak 10062 weight  0.11000E+01 volume  0.10268E+03 ppm1      4.904 ppm2      2.781
ASSI (10072)
  (( segid "BrD " and resid 35   and name HA  ))
  (( segid "BrD " and resid 35   and name HB1 ))
     3.100      2.400      2.400 peak 10072 weight  0.11000E+01 volume  0.86087E+02 ppm1      4.904 ppm2      2.831
ASSI (10112)
  (( segid "BrD " and resid 70   and name HB1 ))
  (  segid "BrD " and resid 69   and name HG2%)
     4.700      4.700      0.800 peak 10112 weight  0.11000E+01 volume  0.77364E+01 ppm1      4.756 ppm2      1.427
ASSI (10122)
  (( segid "BrD " and resid 70   and name HB2 ))
  (  segid "BrD " and resid 69   and name HG2%)
     4.800      4.800      0.700 peak 10122 weight  0.11000E+01 volume  0.67595E+01 ppm1      4.359 ppm2      1.428
ASSI (10132)
  (( segid "BrD " and resid 70   and name HB2 ))
  (  segid "BrD " and resid 69   and name HG1%)
     3.200      2.600      2.300 peak 10132 weight  0.11000E+01 volume  0.71828E+02 ppm1      4.360 ppm2      1.543
ASSI (10232)
  (( segid "BrD " and resid 7    and name HB1 ))
  (( segid "BrD " and resid 7    and name HA  ))
     2.800      2.000      2.000 peak 10232 weight  0.11000E+01 volume  0.15716E+03 ppm1      2.634 ppm2      5.143
ASSI (10242)
  (( segid "BrD " and resid 7    and name HB2 ))
  (( segid "BrD " and resid 7    and name HA  ))
     2.900      2.100      2.100 peak 10242 weight  0.11000E+01 volume  0.13922E+03 ppm1      2.501 ppm2      5.143
ASSI (10252)
  (( segid "BrD " and resid 42   and name HA  ))
  (( segid "BrD " and resid 42   and name HB1 ))
     2.400      1.400      1.400 peak 10252 weight  0.11000E+01 volume  0.37492E+03 ppm1      5.051 ppm2      2.784
ASSI (10292)
  (( segid "BrD " and resid 42   and name HB2 ))
  (( segid "BrD " and resid 42   and name HA  ))
     2.300      1.300      1.300 peak 10292 weight  0.11000E+01 volume  0.48567E+03 ppm1      2.586 ppm2      5.046
ASSI (10312)
  (( segid "BrD " and resid 87   and name HA  ))
  (( segid "BrD " and resid 87   and name HB2 ))
     2.400      1.400      1.400 peak 10312 weight  0.11000E+01 volume  0.37361E+03 ppm1      4.858 ppm2      2.881
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ASSI (10322)
  (( segid "BrD " and resid 87   and name HA  ))
  (( segid "BrD " and resid 87   and name HB1 ))
    2.500     1.600     1.600 peak 10322 weight  0.11000E+01 volume  0.30668E+03 ppm1      4.854 ppm2      2.780
ASSI (10332)
  (( segid "BrD " and resid 87   and name HB1 ))
  (( segid "BrD " and resid 84   and name HA  ))
    2.600     1.700     1.700 peak 10332 weight  0.11000E+01 volume  0.28367E+03 ppm1      2.779 ppm2      4.873
ASSI (10342)
  (( segid "BrD " and resid 87   and name HB2 ))
  (( segid "BrD " and resid 84   and name HA  ))
    2.100     1.100     1.100 peak 10342 weight  0.11000E+01 volume  0.80939E+03 ppm1      2.585 ppm2      4.873
ASSI (10352)
  (( segid "BrD " and resid 87   and name HB2 ))
  (( segid "BrD " and resid 87   and name HG1 ))
    2.300     1.300     1.300 peak 10352 weight  0.11000E+01 volume  0.47273E+03 ppm1      2.585 ppm2      3.021
ASSI (10392)
  (( segid "BrD " and resid 87   and name HG2 ))
  (  segid "BrD " and resid 50   and name HD1% )
    3.500     3.100     2.000 peak 10392 weight  0.11000E+01 volume  0.42729E+02 ppm1      2.782 ppm2      1.145
ASSI (10402)
  (( segid "BrD " and resid 48   and name HA  ))
  (( segid "BrD " and resid 48   and name HB1 ))
    2.400     1.400     1.400 peak 10402 weight  0.11000E+01 volume  0.46141E+03 ppm1      4.803 ppm2      2.729
ASSI (10422)
  (( segid "BrD " and resid 94   and name HA  ))
  (( segid "BrD " and resid 94   and name HB1 ))
    2.300     1.300     1.300 peak 10422 weight  0.11000E+01 volume  0.56402E+03 ppm1      4.831 ppm2      2.731
ASSI (10452)
  (( segid "BrD " and resid 92   and name HB2 ))
  (( segid "BrD " and resid 92   and name HA  ))
    2.300     1.300     1.300 peak 10452 weight  0.11000E+01 volume  0.48724E+03 ppm1      2.570 ppm2      4.798
ASSI (10462)
  (( segid "BrD " and resid 92   and name HB1 ))
  (( segid "BrD " and resid 92   and name HA  ))
    2.000     1.000     1.000 peak 10462 weight  0.11000E+01 volume  0.12901E+04 ppm1      2.694 ppm2      4.798
ASSI (10482)
  (( segid "BrD " and resid 112  and name HB1 ))
  (( segid "BrD " and resid 109  and name HA  ))
    2.400     1.400     1.400 peak 10482 weight  0.11000E+01 volume  0.44320E+03 ppm1      2.684 ppm2      4.638
ASSI (10492)
  (( segid "BrD " and resid 112  and name HB1 ))
  (( segid "BrD " and resid 112  and name HA  ))
    2.400     1.400     1.400 peak 10492 weight  0.11000E+01 volume  0.38447E+03 ppm1      2.684 ppm2      4.587
ASSI (10532)
  (( segid "BrD " and resid 75   and name HA  ))
  (( segid "BrD " and resid 75   and name HB1 ))
    2.500     1.600     1.600 peak 10532 weight  0.11000E+01 volume  0.36144E+03 ppm1      4.509 ppm2      2.931
ASSI (10542)
  (( segid "BrD " and resid 75   and name HA  ))
  (( segid "BrD " and resid 75   and name HB2 ))
    2.400     1.400     1.400 peak 10542 weight  0.11000E+01 volume  0.39358E+03 ppm1      4.509 ppm2      2.847
ASSI (10552)
  (( segid "BrD " and resid 75   and name HG1 ))
  (  segid "BrD " and resid 75   and name HE% )
    2.600     1.700     1.700 peak 10552 weight  0.11000E+01 volume  0.23961E+03 ppm1      3.523 ppm2      2.662
ASSI (10562)
  (( segid "BrD " and resid 75   and name HG2 ))
  (  segid "BrD " and resid 75   and name HE% )
    2.600     1.700     1.700 peak 10562 weight  0.11000E+01 volume  0.23485E+03 ppm1      3.227 ppm2      2.662
ASSI (10632)
  (( segid "BrD " and resid 66   and name HA  ))
  (( segid "BrD " and resid 66   and name HG1 ))
    2.600     1.700     1.700 peak 10632 weight  0.11000E+01 volume  0.25166E+03 ppm1      5.000 ppm2      2.181
ASSI (10642)
  (( segid "BrD " and resid 66   and name HG2 ))
  (( segid "BrD " and resid 66   and name HA  ))
    2.500     1.600     1.600 peak 10642 weight  0.11000E+01 volume  0.30460E+03 ppm1      2.141 ppm2      4.998
ASSI (10652)
  (( segid "BrD " and resid 66   and name HA  ))
  (( segid "BrD " and resid 66   and name HB1 ))
    2.300     1.300     1.300 peak 10652 weight  0.11000E+01 volume  0.48749E+03 ppm1      5.000 ppm2      2.702
ASSI (10662)
  (( segid "BrD " and resid 66   and name HA  ))
  (( segid "BrD " and resid 66   and name HB2 ))
    2.100     1.100     1.100 peak 10662 weight  0.11000E+01 volume  0.87656E+03 ppm1      5.000 ppm2      2.608
ASSI (10672)
  (( segid "BrD " and resid 80   and name HB2 ))
  (( segid "BrD " and resid 77   and name HA  ))
    2.400     1.700     1.700 peak 10672 weight  0.11000E+01 volume  0.24800E+03 ppm1      2.536 ppm2      4.951
ASSI (10682)
  (( segid "BrD " and resid 80   and name HB1 ))
  (( segid "BrD " and resid 77   and name HA  ))
    2.600     1.700     1.700 peak 10682 weight  0.11000E+01 volume  0.24031E+03 ppm1      2.583 ppm2      4.951
ASSI (10692)
  (( segid "BrD " and resid 80   and name HB2 ))
  (( segid "BrD " and resid 80   and name HA  ))
    3.000     2.200     2.200 peak 10692 weight  0.11000E+01 volume  0.11905E+03 ppm1      2.536 ppm2      4.671
ASSI (10702)
  (( segid "BrD " and resid 80   and name HB1 ))
  (( segid "BrD " and resid 80   and name HA  ))
    2.900     2.100     2.100 peak 10702 weight  0.11000E+01 volume  0.13820E+03 ppm1      2.584 ppm2      4.672
ASSI (10752)
  (( segid "BrD " and resid 80   and name HA  ))
  (( segid "BrD " and resid 80   and name HG1 ))
    2.300     1.300     1.300 peak 10752 weight  0.11000E+01 volume  0.52255E+03 ppm1      4.655 ppm2      2.339
ASSI (10762)
  (( segid "BrD " and resid 80   and name HA  ))
  (  segid "BrD " and resid 83   and name HG2% )
    3.200     2.600     2.300 peak 10762 weight  0.11000E+01 volume  0.74619E+02 ppm1      4.655 ppm2      1.901
ASSI (10792)
  (( segid "BrD " and resid 9    and name HA  ))
  (( segid "BrD " and resid 9    and name HB1 ))
    2.500     1.600     1.600 peak 10792 weight  0.11000E+01 volume  0.30562E+03 ppm1      4.953 ppm2      2.424
ASSI (10802)
  (( segid "BrD " and resid 20   and name HA  ))
  (( segid "BrD " and resid 23   and name HB1 ))
    2.800     2.000     2.000 peak 10802 weight  0.11000E+01 volume  0.14886E+03 ppm1      4.901 ppm2      2.931
ASSI (10812)
  (( segid "BrD " and resid 20   and name HA  ))
  (( segid "BrD " and resid 23   and name HB2 ))
    2.900     2.100     2.100 peak 10812 weight  0.11000E+01 volume  0.14118E+03 ppm1      4.901 ppm2      2.857
ASSI (10822)
  (( segid "BrD " and resid 27   and name HB1 ))
  (( segid "BrD " and resid 24   and name HA  ))
    2.500     1.600     1.600 peak 10822 weight  0.11000E+01 volume  0.34604E+03 ppm1      4.608 ppm2      4.788
ASSI (10932)
  (( segid "BrD " and resid 108  and name HA  ))
  (( segid "BrD " and resid 111  and name HB1 ))
    2.900     2.100     2.100 peak 10932 weight  0.11000E+01 volume  0.13575E+03 ppm1      4.801 ppm2      2.475
ASSI (10942)
  (( segid "BrD " and resid 108  and name HA  ))
  (( segid "BrD " and resid 111  and name HB2 ))
    3.000     2.200     2.200 peak 10942 weight  0.11000E+01 volume  0.11676E+03 ppm1      4.803 ppm2      2.351
ASSI (10952)
  (( segid "BrD " and resid 108  and name HA  ))
  (( segid "BrD " and resid 111  and name HD1 ))
    3.200     2.600     2.300 peak 10952 weight  0.11000E+01 volume  0.76235E+02 ppm1      4.803 ppm2      2.237
ASSI (11002)
  (( segid "BrD " and resid 44   and name HG2 ))
  (( segid "BrD " and resid 44   and name HD1 ))
    2.300     1.300     1.300 peak 11002 weight  0.11000E+01 volume  0.53477E+03 ppm1      2.645 ppm2      4.337
ASSI (11032)
  (( segid "BrD " and resid 44   and name HD1 ))
  (( segid "BrD " and resid 43   and name HA  ))
    2.300     1.300     1.300 peak 11032 weight  0.11000E+01 volume  0.59437E+03 ppm1      4.312 ppm2      5.541
ASSI (11092)
  (( segid "BrD " and resid 11   and name HA  ))
  (( segid "BrD " and resid 14   and name HB1 ))
    3.000     2.200     2.200 peak 11092 weight  0.11000E+01 volume  0.11894E+03 ppm1      4.951 ppm2      2.471
ASSI (11112)
  (( segid "BrD " and resid 11   and name HD1 ))
  (( segid "BrD " and resid 10   and name HB2 ))
    2.800     2.000     2.000 peak 11112 weight  0.11000E+01 volume  0.15710E+03 ppm1      4.457 ppm2      3.300
ASSI (11122)
  (( segid "BrD " and resid 11   and name HD1 ))
  (( segid "BrD " and resid 10   and name HB1 ))
    3.000     2.200     2.200 peak 11122 weight  0.11000E+01 volume  0.11776E+03 ppm1      4.457 ppm2      3.355
ASSI (11152)
  (( segid "BrD " and resid 37   and name HD1 ))
  (( segid "BrD " and resid 36   and name HA  ))
    3.400     2.900     2.100 peak 11152 weight  0.11000E+01 volume  0.48585E+02 ppm1      4.262 ppm2      5.446
ASSI (11182)
  (( segid "BrD " and resid 53   and name HD2 ))
  (  segid "BrD " and resid 50   and name HG2% )
    3.400     2.900     2.100 peak 11182 weight  0.11000E+01 volume  0.47917E+02 ppm1      4.015 ppm2      0.993
ASSI (11212)
  (( segid "BrD " and resid 53   and name HG1 ))
  (( segid "BrD " and resid 53   and name HD1 ))
    2.800     2.000     2.000 peak 11212 weight  0.11000E+01 volume  0.15118E+03 ppm1      2.784 ppm2      4.209
ASSI (11222)
  (( segid "BrD " and resid 53   and name HG2 ))
  (( segid "BrD " and resid 53   and name HD1 ))
    2.800     2.000     2.000 peak 11222 weight  0.11000E+01 volume  0.15165E+03 ppm1      2.490 ppm2      4.210
ASSI (11232)
  (( segid "BrD " and resid 53   and name HG2 ))
  (( segid "BrD " and resid 53   and name HD2 ))
    2.900     2.100     2.100 peak 11232 weight  0.11000E+01 volume  0.12572E+03 ppm1      2.488 ppm2      4.011
ASSI (11242)
  (( segid "BrD " and resid 53   and name HG1 ))
  (( segid "BrD " and resid 53   and name HD2 ))
    3.100     2.400     2.400 peak 11242 weight  0.11000E+01 volume  0.94017E+02 ppm1      2.784 ppm2      4.011
ASSI (11252)
  (( segid "BrD " and resid 53   and name HG1 ))
  (  segid "BrD " and resid 50   and name HG2% )
    4.300     4.300     1.200 peak 11252 weight  0.11000E+01 volume  0.13261E+02 ppm1      2.784 ppm2      0.993
ASSI (11272)
  (( segid "BrD " and resid 19   and name HB1 ))
  (  segid "BrD " and resid 63   and name HD2% )
    3.000     2.200     2.200 peak 11272 weight  0.11000E+01 volume  0.10292E+03 ppm1      2.290 ppm2      1.492
ASSI (11292)
  (( segid "BrD " and resid 19   and name HB1 ))
  (  segid "BrD " and resid 63   and name HD1% )
    3.300     2.700     2.200 peak 11292 weight  0.11000E+01 volume  0.56479E+02 ppm1      2.290 ppm2      1.655
ASSI (11302)
  (( segid "BrD " and resid 19   and name HB2 ))
  (  segid "BrD " and resid 63   and name HD1% )
    3.400     2.900     2.100 peak 11302 weight  0.11000E+01 volume  0.52899E+02 ppm1      1.988 ppm2      1.655
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ASSI (11392)
   (( segid "BrD " and resid 97   and name HA  ))
   (( segid "BrD " and resid 97   and name HG1 ))
     2.400     1.400     1.400 peak 11392 weight  0.11000E+01 volume  0.40873E+03 ppm1      4.805 ppm2      2.438
ASSI (11422)
   (( segid "BrD " and resid 97   and name HB1 ))
   (( segid "BrD " and resid 94   and name HA  ))
     2.200     1.200     1.200 peak 11422 weight  0.11000E+01 volume  0.64841E+03 ppm1      2.685 ppm2      4.830
ASSI (11442)
   (( segid "BrD " and resid 97   and name HD1 ))
   (( segid "BrD " and resid 97   and name HA  ))
     3.600     3.200     1.900 peak 11442 weight  0.11000E+01 volume  0.36224E+03 ppm1      2.420 ppm2      4.800
ASSI (11472)
   (( segid "BrD " and resid 86   and name HB1 ))
   (( segid "BrD " and resid 86   and name HA  ))
     2.400     1.400     1.400 peak 11472 weight  0.11000E+01 volume  0.38167E+03 ppm1      2.360 ppm2      4.807
ASSI (11482)
   (( segid "BrD " and resid 86   and name HB1 ))
   (( segid "BrD " and resid 86   and name HG2 ))
     2.900     2.100     2.100 peak 11482 weight  0.11000E+01 volume  0.12261E+03 ppm1      2.360 ppm2      0.766
ASSI (11612)
   (( segid "BrD " and resid 64   and name HB1 ))
   (( segid "BrD " and resid 61   and name HA  ))
     2.300     1.300     1.300 peak 11612 weight  0.11000E+01 volume  0.48201E+03 ppm1      2.636 ppm2      4.667
ASSI (11622)
   (( segid "BrD " and resid 64   and name HG1 ))
   (( segid "BrD " and resid 61   and name HA  ))
     2.600     1.700     1.700 peak 11622 weight  0.11000E+01 volume  0.27263E+03 ppm1      2.190 ppm2      4.667
ASSI (11692)
   (( segid "BrD " and resid 6    and name HA  ))
   (( segid "BrD " and resid 6    and name HB2 ))
     2.400     1.400     1.400 peak 11692 weight  0.11000E+01 volume  0.40526E+03 ppm1      4.972 ppm2      2.291
ASSI (11702)
   (( segid "BrD " and resid 72   and name HD1 ))
   (( segid "BrD " and resid 72   and name HA  ))
     2.600     1.700     1.700 peak 11702 weight  0.11000E+01 volume  0.26243E+03 ppm1      2.291 ppm2      4.646
ASSI (11712)
   (( segid "BrD " and resid 62   and name HD1 ))
   (( segid "BrD " and resid 62   and name HG1 ))
     2.700     1.800     1.800 peak 11712 weight  0.11000E+01 volume  0.19040E+03 ppm1      3.177 ppm2      2.323
ASSI (11732)
   (( segid "BrD " and resid 62   and name HD2 ))
   (( segid "BrD " and resid 62   and name HG2 ))
     3.200     2.600     2.300 peak 11732 weight  0.11000E+01 volume  0.69523E+02 ppm1      2.629 ppm2      1.480
ASSI (11742)
   (( segid "BrD " and resid 62   and name HD1 ))
   (( segid "BrD " and resid 59   and name HA  ))
     3.100     2.400     2.400 peak 11742 weight  0.11000E+01 volume  0.81736E+02 ppm1      3.177 ppm2      4.911
ASSI (11782)
   (( segid "BrD " and resid 91   and name HG1 ))
   (( segid "BrD " and resid 91   and name HD2 ))
     3.000     2.200     2.200 peak 11782 weight  0.11000E+01 volume  0.11953E+03 ppm1      2.779 ppm2      4.406
ASSI (11802)
   (( segid "BrD " and resid 91   and name HA  ))
   (( segid "BrD " and resid 91   and name HB1 ))
     2.700     1.800     1.800 peak 11802 weight  0.11000E+01 volume  0.18443E+03 ppm1      5.347 ppm2      2.978
ASSI (11812)
   (( segid "BrD " and resid 91   and name HA  ))
   (( segid "BrD " and resid 91   and name HG1 ))
     3.700     3.400     1.800 peak 11812 weight  0.11000E+01 volume  0.32384E+02 ppm1      5.347 ppm2      2.788
ASSI (11852)
   (( segid "BrD " and resid 91   and name HD1 ))
   (( segid "BrD " and resid 89   and name HA  ))
     2.700     1.800     1.800 peak 11852 weight  0.11000E+01 volume  0.19122E+03 ppm1      4.559 ppm2      5.642
ASSI (11882)
   (( segid "BrD " and resid 91   and name HD2 ))
   (( segid "BrD " and resid 89   and name HB1 ))
     2.800     2.000     2.000 peak 11882 weight  0.11000E+01 volume  0.16587E+03 ppm1      4.410 ppm2      3.668
ASSI (11912)
   (( segid "BrD " and resid 91   and name HB2 ))
   (( segid "BrD " and resid 91   and name HD1 ))
     3.700     3.400     1.800 peak 11912 weight  0.11000E+01 volume  0.31825E+02 ppm1      2.730 ppm2      4.559
ASSI (11922)
   (( segid "BrD " and resid 91   and name HB1 ))
   (( segid "BrD " and resid 91   and name HD1 ))
     3.400     2.900     2.100 peak 11922 weight  0.11000E+01 volume  0.50256E+02 ppm1      2.978 ppm2      4.559
ASSI (11942)
   (( segid "BrD " and resid 91   and name HB2 ))
   (( segid "BrD " and resid 91   and name HA  ))
     2.800     2.000     2.000 peak 11942 weight  0.11000E+01 volume  0.17033E+03 ppm1      2.725 ppm2      5.378
ASSI (11952)
   (( segid "BrD " and resid 33   and name HA  ))
   (( segid "BrD " and resid 33   and name HG2 ))
     3.000     2.200     2.200 peak 11952 weight  0.11000E+01 volume  0.10731E+03 ppm1      4.361 ppm2     -0.319
ASSI (11962)
   (( segid "BrD " and resid 33   and name HA  ))
   (( segid "BrD " and resid 33   and name HB2 ))
     2.700     1.800     1.800 peak 11962 weight  0.11000E+01 volume  0.20069E+03 ppm1      4.361 ppm2     -0.166
ASSI (11972)
   (( segid "BrD " and resid 33   and name HA  ))
   (( segid "BrD " and resid 33   and name HB1 ))
     2.700     1.800     1.800 peak 11972 weight  0.11000E+01 volume  0.18669E+03 ppm1      4.360 ppm2      1.083
ASSI (12032)
   (( segid "BrD " and resid 33   and name HG1 ))
   (( segid "BrD " and resid 33   and name HB2 ))
     2.900     2.100     2.100 peak 12032 weight  0.11000E+01 volume  0.13883E+03 ppm1      0.858 ppm2     -0.165
ASSI (12042)
   (( segid "BrD " and resid 33   and name HG2 ))
   (( segid "BrD " and resid 33   and name HB2 ))
     2.900     2.100     2.100 peak 12042 weight  0.11000E+01 volume  0.12386E+03 ppm1     -0.324 ppm2     -0.169
ASSI (12062)
   (( segid "BrD " and resid 33   and name HD1 ))
   (( segid "BrD " and resid 33   and name HG1 ))
     3.000     2.200     2.200 peak 12062 weight  0.11000E+01 volume  0.11534E+03 ppm1      2.780 ppm2      0.864
ASSI (12072)
   (( segid "BrD " and resid 33   and name HD2 ))
   (( segid "BrD " and resid 33   and name HG1 ))
     3.100     2.400     2.400 peak 12072 weight  0.11000E+01 volume  0.97683E+02 ppm1      2.189 ppm2      0.864
ASSI (12082)
   (( segid "BrD " and resid 33   and name HD1 ))
   (( segid "BrD " and resid 33   and name HG2 ))
     2.900     2.100     2.100 peak 12082 weight  0.11000E+01 volume  0.13243E+03 ppm1      2.780 ppm2     -0.319
ASSI (12092)
   (( segid "BrD " and resid 33   and name HD2 ))
   (( segid "BrD " and resid 33   and name HG2 ))
     2.900     2.100     2.100 peak 12092 weight  0.11000E+01 volume  0.13995E+03 ppm1      2.189 ppm2     -0.319
ASSI (12102)
   (( segid "BrD " and resid 33   and name HB1 ))
   (( segid "BrD " and resid 33   and name HG2 ))
     2.900     2.100     2.100 peak 12102 weight  0.11000E+01 volume  0.14146E+03 ppm1      1.051 ppm2     -0.316
ASSI (12132)
   (( segid "BrD " and resid 33   and name HB1 ))
   (( segid "BrD " and resid 33   and name HD1 ))
     3.100     2.400     2.400 peak 12132 weight  0.11000E+01 volume  0.94208E+02 ppm1      1.089 ppm2      0.889
ASSI (12182)
   (( segid "BrD " and resid 35   and name HA  ))
   (( segid "BrD " and resid 36   and name HB1 ))
     4.100     4.100     1.400 peak 12182 weight  0.11000E+01 volume  0.16299E+02 ppm1      4.904 ppm2      2.685
ASSI (12222)
   (( segid "BrD " and resid 59   and name HG2 ))
   (  segid "BrD " and resid 59   and name HE% )
     2.300     1.300     1.300 peak 12222 weight  0.11000E+01 volume  0.52760E+03 ppm1      3.137 ppm2      1.875
ASSI (12242)
   (( segid "BrD " and resid 59   and name HB2 ))
   (  segid "BrD " and resid 59   and name HE% )
     2.700     1.800     1.800 peak 12242 weight  0.11000E+01 volume  0.19334E+03 ppm1      2.487 ppm2      1.876
ASSI (12252)
   (( segid "BrD " and resid 59   and name HA  ))
   (( segid "BrD " and resid 59   and name HB2 ))
     3.300     2.700     2.200 peak 12252 weight  0.11000E+01 volume  0.59031E+02 ppm1      4.903 ppm2      2.487
ASSI (12262)
   (( segid "BrD " and resid 59   and name HA  ))
   (( segid "BrD " and resid 62   and name HB1 ))
     3.100     2.400     2.400 peak 12262 weight  0.11000E+01 volume  0.90578E+02 ppm1      4.903 ppm2      2.657
ASSI (12272)
   (( segid "BrD " and resid 59   and name HA  ))
   (( segid "BrD " and resid 62   and name HB2 ))
     2.900     2.100     2.100 peak 12272 weight  0.11000E+01 volume  0.13057E+03 ppm1      4.903 ppm2      1.670
ASSI (12312)
   (( segid "BrD " and resid 61   and name HB1 ))
   (( segid "BrD " and resid 61   and name HA  ))
     2.500     1.600     1.600 peak 12312 weight  0.11000E+01 volume  0.30078E+03 ppm1      2.826 ppm2      4.673
ASSI (12322)
   (( segid "BrD " and resid 61   and name HB1 ))
   (( segid "BrD " and resid 58   and name HA  ))
     3.000     2.200     2.200 peak 12322 weight  0.11000E+01 volume  0.10836E+03 ppm1      2.826 ppm2      4.451
ASSI (12332)
   (( segid "BrD " and resid 61   and name HB2 ))
   (( segid "BrD " and resid 58   and name HA  ))
     2.400     1.400     1.400 peak 12332 weight  0.11000E+01 volume  0.42931E+03 ppm1      2.679 ppm2      4.451
ASSI (12342)
   (( segid "BrD " and resid 61   and name HB2 ))
   (( segid "BrD " and resid 61   and name HA  ))
     2.100     1.100     1.100 peak 12342 weight  0.11000E+01 volume  0.81117E+03 ppm1      2.679 ppm2      4.673
ASSI (12392)
   (  segid "BrD " and resid 102  and name HD2% )
   (( segid "BrD " and resid 102  and name HG  ))
     2.000     1.000     1.000 peak 12392 weight  0.11000E+01 volume  0.13682E+04 ppm1      1.304 ppm2      2.159
ASSI (12402)
   (  segid "BrD " and resid 102  and name HD2% )
   (( segid "BrD " and resid 102  and name HB1 ))
     2.400     1.400     1.400 peak 12402 weight  0.11000E+01 volume  0.42022E+03 ppm1      1.304 ppm2      2.020
ASSI (12422)
   (  segid "BrD " and resid 102  and name HD2% )
   (  segid "BrD " and resid 31   and name HB% )
     3.500     3.100     2.000 peak 12422 weight  0.11000E+01 volume  0.40319E+02 ppm1      1.305 ppm2      2.315
ASSI (12432)
   (  segid "BrD " and resid 14   and name HD1% )
   (( segid "BrD " and resid 14   and name HG  ))
     2.400     1.400     1.400 peak 12432 weight  0.11000E+01 volume  0.38368E+03 ppm1      1.402 ppm2      2.062
ASSI (12442)
   (  segid "BrD " and resid 14   and name HD1% )
   (( segid "BrD " and resid 14   and name HB2 ))
     2.300     1.300     1.300 peak 12442 weight  0.11000E+01 volume  0.51224E+03 ppm1      1.402 ppm2      2.185
ASSI (12452)
   (  segid "BrD " and resid 14   and name HD1% )
   (( segid "BrD " and resid 14   and name HB1 ))
     2.300     1.300     1.300 peak 12452 weight  0.11000E+01 volume  0.51311E+03 ppm1      1.402 ppm2      2.468
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ASSI (12462)
  ( segid "BrD " and resid 14   and name HD1%)
  (( segid "BrD " and resid 14   and name HA  ))
     2.600     1.700     1.700 peak 12462 weight  0.11000E+01 volume  0.23971E+03 ppm1     1.401 ppm2     4.655
ASSI (12472)
  ( segid "BrD " and resid 14   and name HD1%)
  ( segid "BrD " and resid 18   and name HD1%)
     2.500     1.600     1.600 peak 12472 weight  0.11000E+01 volume  0.29352E+03 ppm1     1.402 ppm2     1.084
ASSI (12602)
  ( segid "BrD " and resid 59   and name HE% )
  (( segid "BrD " and resid 59   and name HB1 ))
     2.700     1.800     1.800 peak 12602 weight  0.11000E+01 volume  0.21211E+03 ppm1     1.847 ppm2     2.707
ASSI (12622)
  ( segid "BrD " and resid 59   and name HE% )
  (( segid "BrD " and resid 59   and name HG1 ))
     3.100     2.400     2.400 peak 12622 weight  0.11000E+01 volume  0.88634E+02 ppm1     1.848 ppm2     3.230
ASSI (12662)
  ( segid "BrD " and resid 54   and name HE% )
  (( segid "BrD " and resid 54   and name HB2 ))
     2.700     1.800     1.800 peak 12662 weight  0.11000E+01 volume  0.21213E+03 ppm1     2.535 ppm2     1.964
ASSI (12682)
  ( segid "BrD " and resid 54   and name HE% )
  (( segid "BrD " and resid 54   and name HG1 ))
     2.500     1.600     1.600 peak 12682 weight  0.11000E+01 volume  0.35414E+03 ppm1     2.535 ppm2     3.307
ASSI (12772)
  ( segid "BrD " and resid 50   and name HG2%)
  (( segid "BrD " and resid 84   and name HB1 ))
     2.900     2.100     2.100 peak 12772 weight  0.11000E+01 volume  0.14057E+03 ppm1     1.004 ppm2     3.605
ASSI (12802)
  (( segid "BrD " and resid 78   and name HB2 ))
  (( segid "BrD " and resid 75   and name HA  ))
     3.300     2.700     2.200 peak 12802 weight  0.11000E+01 volume  0.66311E+02 ppm1     1.054 ppm2     4.517
ASSI (12902)
  ( segid "BrD " and resid 38   and name HG1%)
  ( segid "BrD " and resid 43   and name HB% )
     2.800     2.000     2.000 peak 12902 weight  0.11000E+01 volume  0.17186E+03 ppm1     1.059 ppm2     1.715
ASSI (12912)
  (( segid "BrD " and resid 25   and name HA  ))
  (( segid "BrD " and resid 28   and name HB2 ))
     3.400     2.900     2.100 peak 12912 weight  0.11000E+01 volume  0.50976E+02 ppm1     4.412 ppm2     3.406
ASSI (12922)
  (( segid "BrD " and resid 25   and name HA  ))
  (( segid "BrD " and resid 28   and name HB1 ))
     3.400     2.900     2.100 peak 12922 weight  0.11000E+01 volume  0.50633E+02 ppm1     4.412 ppm2     3.607
ASSI (12932)
  (( segid "BrD " and resid 25   and name HB  ))
  (( segid "BrD " and resid 25   and name HA  ))
     2.600     1.700     1.700 peak 12932 weight  0.11000E+01 volume  0.25503E+03 ppm1     2.979 ppm2     4.436
ASSI (12942)
  (( segid "BrD " and resid 99   and name HA  ))
  ( segid "BrD " and resid 102  and name HD1%)
     3.500     3.100     2.000 peak 12942 weight  0.11000E+01 volume  0.42963E+02 ppm1     4.458 ppm2     1.321
ASSI (12952)
  ( segid "BrD " and resid 17   and name HG2%)
  ( segid "BrD " and resid 18   and name HD1%)
     3.100     2.400     2.400 peak 12952 weight  0.11000E+01 volume  0.90746E+02 ppm1     1.745 ppm2     1.083
ASSI (12982)
  (( segid "BrD " and resid 98   and name HB1 ))
  (( segid "BrD " and resid 95   and name HA  ))
     3.200     2.600     2.300 peak 12982 weight  0.11000E+01 volume  0.76248E+02 ppm1     4.013 ppm2     4.445
ASSI (13062)
  ( segid "BrD " and resid 56   and name HD1%)
  (( segid "BrD " and resid 34   and name HB2 ))
     2.900     2.100     2.100 peak 13062 weight  0.11000E+01 volume  0.13096E+03 ppm1     1.546 ppm2     3.143
ASSI (13152)
  (( segid "BrD " and resid 81   and name HA  ))
  (( segid "BrD " and resid 84   and name HB2 ))
     3.300     2.700     2.200 peak 13152 weight  0.11000E+01 volume  0.59764E+02 ppm1     3.718 ppm2     3.278
ASSI (13162)
  (( segid "BrD " and resid 85   and name HA  ))
  (( segid "BrD " and resid 88   and name HB1 ))
     3.400     2.900     2.100 peak 13162 weight  0.11000E+01 volume  0.52965E+02 ppm1     5.003 ppm2     3.532
ASSI (13172)
  (( segid "BrD " and resid 86   and name HB1 ))
  (( segid "BrD " and resid 83   and name HA  ))
     3.700     3.400     1.800 peak 13172 weight  0.11000E+01 volume  0.32755E+02 ppm1     2.340 ppm2     4.462
ASSI (13182)
  ( segid "BrD " and resid 54   and name HE% )
  (( segid "BrD " and resid 54   and name HA  ))
     2.300     1.300     1.300 peak 13182 weight  0.11000E+01 volume  0.48303E+03 ppm1     2.535 ppm2     5.543
ASSI (13212)
  (( segid "BrD " and resid 47   and name HA  ))
  (( segid "BrD " and resid 50   and name HB  ))
     3.600     3.200     1.900 peak 13212 weight  0.11000E+01 volume  0.37838E+02 ppm1     4.704 ppm2     1.823
ASSI (13222)
  ( segid "BrD " and resid 81   and name HG2%)
  (( segid "BrD " and resid 34   and name HB2 ))
     2.800     2.000     2.000 peak 13222 weight  0.11000E+01 volume  0.16892E+03 ppm1     0.756 ppm2     3.149
ASSI (13252)
  (( segid "BrD " and resid 34   and name HB2 ))
  (( segid "BrD " and resid 56   and name HG  ))
     3.100     2.400     2.400 peak 13252 weight  0.11000E+01 volume  0.87944E+02 ppm1     3.127 ppm2     2.323
ASSI (13262)
  (( segid "BrD " and resid 34   and name HB1 ))
  (( segid "BrD " and resid 56   and name HG  ))
     3.200     3.600     2.300 peak 13262 weight  0.11000E+01 volume  0.75137E+02 ppm1     4.108 ppm2     2.322
ASSI (13362)
  ( segid "BrD " and resid 18   and name HD1%)
  (( segid "BrD " and resid 18   and name HB1 ))
     2.300     1.300     1.300 peak 13362 weight  0.11000E+01 volume  0.50793E+03 ppm1     1.058 ppm2     2.128
ASSI (13372)
  (( segid "BrD " and resid 14   and name HB1 ))
  ( segid "BrD " and resid 18   and name HD1%)
     4.000     4.000     1.500 peak 13372 weight  0.11000E+01 volume  0.18693E+02 ppm1     2.441 ppm2     1.084
ASSI (13382)
  ( segid "BrD " and resid 25   and name HG1%)
  (( segid "BrD " and resid 22   and name HA  ))
     2.600     1.700     1.700 peak 13382 weight  0.11000E+01 volume  0.28896E+03 ppm1     1.795 ppm2     4.720
ASSI (13402)
  (( segid "BrD " and resid 102  and name HB2 ))
  (( segid "BrD " and resid 99   and name HA  ))
     2.600     1.700     1.700 peak 13402 weight  0.11000E+01 volume  0.26245E+03 ppm1     1.842 ppm2     4.441
ASSI (13422)
  (( segid "BrD " and resid 21   and name HB  ))
  ( segid "BrD " and resid 18   and name HD2%)
     3.700     3.400     1.800 peak 13422 weight  0.11000E+01 volume  0.29780E+02 ppm1     2.487 ppm2     0.409
ASSI (13432)
  (( segid "BrD " and resid 57   and name HA  ))
  (( segid "BrD " and resid 60   and name HB2 ))
     2.700     1.800     1.800 peak 13432 weight  0.11000E+01 volume  0.19090E+03 ppm1     4.805 ppm2     4.625
ASSI (13442)
  (( segid "BrD " and resid 57   and name HA  ))
  (( segid "BrD " and resid 60   and name HB1 ))
     2.900     2.100     2.100 peak 13442 weight  0.11000E+01 volume  0.14250E+03 ppm1     4.805 ppm2     5.000
ASSI (13482)
  ( segid "BrD " and resid 58   and name HG2%)
  (( segid "BrD " and resid 62   and name HD2 ))
     2.800     2.000     2.000 peak 13482 weight  0.11000E+01 volume  0.17578E+03 ppm1     1.651 ppm2     2.644
ASSI (13492)
  (( segid "BrD " and resid 61   and name HB1 ))
  ( segid "BrD " and resid 58   and name HG2%)
     3.600     3.200     1.900 peak 13492 weight  0.11000E+01 volume  0.34592E+02 ppm1     2.826 ppm2     1.662
ASSI (13512)
  ( segid "BrD " and resid 59   and name HE% )
  (( segid "BrD " and resid 59   and name HA  ))
     3.100     2.400     2.400 peak 13512 weight  0.11000E+01 volume  0.83827E+02 ppm1     1.848 ppm2     4.913
ASSI (13522)
  ( segid "BrD " and resid 59   and name HE% )
  ( segid "BrD " and resid 56   and name HD2%)
     3.400     2.900     2.100 peak 13522 weight  0.11000E+01 volume  0.55813E+02 ppm1     1.848 ppm2     1.271
ASSI (13542)
  (( segid "BrD " and resid 21   and name HA  ))
  (( segid "BrD " and resid 24   and name HB2 ))
     3.200     2.600     2.300 peak 13542 weight  0.11000E+01 volume  0.69544E+02 ppm1     4.360 ppm2     2.989
ASSI (13552)
  (( segid "BrD " and resid 74   and name HB2 ))
  (( segid "BrD " and resid 71   and name HA  ))
     3.300     2.700     2.200 peak 13552 weight  0.11000E+01 volume  0.56669E+02 ppm1     2.974 ppm2     4.624
ASSI (13652)
  ( segid "BrD " and resid 58   and name HG2%)
  (( segid "BrD " and resid 62   and name HD1 ))
     2.800     2.000     2.000 peak 13652 weight  0.11000E+01 volume  0.18084E+03 ppm1     1.649 ppm2     1.182
ASSI (13662)
  (( segid "BrD " and resid 32   and name HA  ))
  ( segid "BrD " and resid 31   and name HB% )
     3.700     3.400     1.800 peak 13662 weight  0.11000E+01 volume  0.29321E+02 ppm1     4.952 ppm2     2.312
ASSI (13702)
  (( segid "BrD " and resid 42   and name HB1 ))
  ( segid "BrD " and resid 43   and name HB% )
     3.800     3.600     1.700 peak 13702 weight  0.11000E+01 volume  0.26752E+02 ppm1     2.785 ppm2     1.712
ASSI (13722)
  (( segid "BrD " and resid 59   and name HA  ))
  (( segid "BrD " and resid 62   and name HD2 ))
     2.600     1.700     1.700 peak 13722 weight  0.11000E+01 volume  0.25810E+03 ppm1     4.903 ppm2     2.634
ASSI (13742)
  (( segid "BrD " and resid 63   and name HG  ))
  (( segid "BrD " and resid 63   and name HB1 ))
     2.300     1.300     1.300 peak 13742 weight  0.11000E+01 volume  0.59564E+03 ppm1     2.437 ppm2     2.905
ASSI (13902)
  (( segid "BrD " and resid 70   and name HB1 ))
  ( segid "BrD " and resid 69   and name HG1%)
     3.700     3.400     1.800 peak 13902 weight  0.11000E+01 volume  0.30896E+02 ppm1     4.756 ppm2     1.544
ASSI (13912)
  ( segid "BrD " and resid 101  and name HG2%)
  (( segid "BrD " and resid 98   and name HA  ))
     2.800     2.000     2.000 peak 13912 weight  0.11000E+01 volume  0.17496E+03 ppm1     1.596 ppm2     4.810
ASSI (13932)
  (( segid "BrD " and resid 101  and name HG12))
  (( segid "BrD " and resid 98   and name HA  ))
     3.400     2.900     2.100 peak 13932 weight  0.11000E+01 volume  0.55145E+02 ppm1     1.797 ppm2     4.808
ASSI (13942)
  (( segid "BrD " and resid 98   and name HA  ))
  (( segid "BrD " and resid 101  and name HG11))
     3.200     2.700     2.200 peak 13942 weight  0.11000E+01 volume  0.65568E+02 ppm1     4.804 ppm2     2.469
ASSI (14002)
  (( segid "BrD " and resid 53   and name HB1 ))
  (( segid "BrD " and resid 53   and name HD1 ))
     2.800     2.000     2.000 peak 14002 weight  0.11000E+01 volume  0.16043E+03 ppm1     2.781 ppm2     4.208
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ASSI (14012)
  (( segid "BrD " and resid 53   and name HB1 ))
  (( segid "BrD " and resid 53   and name HD2 ))
     3.000     2.200     2.200 peak 14012 weight  0.11000E+01 volume  0.10929E+03 ppm1      2.781 ppm2      4.010
ASSI (14072)
  (( segid "BrD " and resid 79   and name HA ))
  (( segid "BrD " and resid 82   and name HB2 ))
     3.000     2.200     2.200 peak 14072 weight  0.11000E+01 volume  0.11123E+03 ppm1      4.409 ppm2      3.606
ASSI (14082)
  (( segid "BrD " and resid 79   and name HA ))
  (( segid "BrD " and resid 82   and name HB1 ))
     3.300     2.700     2.200 peak 14082 weight  0.11000E+01 volume  0.67314E+02 ppm1      4.409 ppm2      3.697
ASSI (14092)
  (( segid "BrD " and resid 79   and name HB2 ))
  (( segid "BrD " and resid 76   and name HA ))
     2.400     1.400     1.400 peak 14092 weight  0.11000E+01 volume  0.38186E+03 ppm1      2.680 ppm2      4.683
ASSI (14182)
  (( segid "BrD " and resid 94   and name HA ))
  (( segid "BrD " and resid 97   and name HD1 ))
     3.200     2.600     2.300 peak 14182 weight  0.11000E+01 volume  0.68636E+02 ppm1      4.830 ppm2      2.434
ASSI (14252)
  (( segid "BrD " and resid 113  and name HA ))
  (  segid "BrD " and resid 17   and name HG2%)
     3.600     3.200     1.900 peak 14252 weight  0.11000E+01 volume  0.37471E+02 ppm1      4.901 ppm2      1.750
ASSI (14552)
  (( segid "BrD " and resid 11   and name HB2 ))
  (( segid "BrD " and resid 11   and name HD1 ))
     2.700     1.800     1.800 peak 14552 weight  0.11000E+01 volume  0.21551E+03 ppm1      2.580 ppm2      4.460
ASSI (14572)
  (( segid "BrD " and resid 14   and name HB2 ))
  (( segid "BrD " and resid 11   and name HA ))
     3.300     2.700     2.200 peak 14572 weight  0.11000E+01 volume  0.58722E+02 ppm1      2.145 ppm2      4.942
ASSI (14592)
  (  segid "BrD " and resid 102  and name HD2%)
  (( segid "BrD " and resid 31   and name HA ))
     3.400     2.900     2.100 peak 14592 weight  0.11000E+01 volume  0.51768E+02 ppm1      1.303 ppm2      4.984
ASSI (14612)
  (  segid "BrD " and resid 102  and name HD2%)
  (  segid "BrD " and resid 25   and name HG2%)
     2.300     1.300     1.300 peak 14612 weight  0.11000E+01 volume  0.50747E+03 ppm1      1.305 ppm2      1.633
ASSI (14622)
  (  segid "BrD " and resid 102  and name HD2%)
  (( segid "BrD " and resid 25   and name HA ))
     2.700     1.800     1.800 peak 14622 weight  0.11000E+01 volume  0.22785E+03 ppm1      1.303 ppm2      4.425
ASSI (14662)
  (( segid "BrD " and resid 18   and name HB2 ))
  (( segid "BrD " and resid 18   and name HG  ))
     3.100     2.400     2.400 peak 14662 weight  0.11000E+01 volume  0.98623E+02 ppm1      0.911 ppm2      2.274
ASSI (14772)
  (( segid "BrD " and resid 36   and name HA ))
  (( segid "BrD " and resid 37   and name HG2 ))
     5.500     5.500     0.000 peak 14772 weight  0.11000E+01 volume  0.48374E+00 ppm1      5.447 ppm2      2.587
ASSI (14812)
  (( segid "BrD " and resid 42   and name HB2 ))
  (  segid "BrD " and resid 43   and name HB% )
     3.200     2.600     2.300 peak 14812 weight  0.11000E+01 volume  0.74053E+02 ppm1      2.586 ppm2      1.710
ASSI (14822)
  (( segid "BrD " and resid 35   and name HA ))
  (( segid "BrD " and resid 36   and name HB2 ))
     3.800     3.600     1.700 peak 14822 weight  0.11000E+01 volume  0.27804E+02 ppm1      4.904 ppm2      2.340
ASSI (14942)
  (( segid "BrD " and resid 46   and name HA ))
  (  segid "BrD " and resid 88   and name HE% )
     2.700     1.800     1.800 peak 14942 weight  0.11000E+01 volume  0.19889E+03 ppm1      4.163 ppm2      7.421
ASSI (14962)
  (( segid "BrD " and resid 46   and name HA ))
  (  segid "BrD " and resid 46   and name HE% )
     3.600     3.200     1.900 peak 14962 weight  0.11000E+01 volume  0.36218E+02 ppm1      4.164 ppm2      6.689
ASSI (14992)
  (( segid "BrD " and resid 46   and name HB2 ))
  (  segid "BrD " and resid 46   and name HE% )
     3.700     3.400     1.800 peak 14992 weight  0.11000E+01 volume  0.28675E+02 ppm1      3.078 ppm2      6.689
ASSI (15062)
  (( segid "BrD " and resid 28   and name HB2 ))
  (( segid "BrD " and resid 28   and name HD2 ))
     3.100     2.400     2.400 peak 15062 weight  0.11000E+01 volume  0.98530E+02 ppm1      3.372 ppm2      5.575
ASSI (15072)
  (( segid "BrD " and resid 28   and name HB1 ))
  (( segid "BrD " and resid 28   and name HD2 ))
     3.200     2.600     2.300 peak 15072 weight  0.11000E+01 volume  0.74212E+02 ppm1      3.570 ppm2      5.575
ASSI (15122)
  (( segid "BrD " and resid 67   and name HB1 ))
  (  segid "BrD " and resid 67   and name HE% )
     4.100     4.100     1.400 peak 15122 weight  0.11000E+01 volume  0.17734E+02 ppm1      2.639 ppm2      7.315
ASSI (15292)
  (( segid "BrD " and resid 47   and name HA ))
  (  segid "BrD " and resid 46   and name HD% )
     4.100     4.100     1.400 peak 15292 weight  0.11000E+01 volume  0.16402E+02 ppm1      4.705 ppm2      5.762
ASSI (15322)
  (( segid "BrD " and resid 47   and name HB2 ))
  (  segid "BrD " and resid 47   and name HE% )
     3.400     2.900     2.100 peak 15322 weight  0.11000E+01 volume  0.56146E+02 ppm1      3.378 ppm2      7.271
ASSI (15332)
  (( segid "BrD " and resid 47   and name HB1 ))
  (  segid "BrD " and resid 47   and name HE% )
     3.200     2.600     2.300 peak 15332 weight  0.11000E+01 volume  0.74345E+02 ppm1      3.816 ppm2      7.271
ASSI (15352)
  (( segid "BrD " and resid 32   and name HB2 ))
  (( segid "BrD " and resid 32   and name HE3 ))
     2.600     1.700     1.700 peak 15352 weight  0.11000E+01 volume  0.27498E+03 ppm1      3.962 ppm2      7.952
ASSI (15432)
  (( segid "BrD " and resid 74   and name HB1 ))
  (  segid "BrD " and resid 74   and name HD% )
     2.900     2.100     2.100 peak 15432 weight  0.11000E+01 volume  0.14689E+03 ppm1      3.576 ppm2      6.998
ASSI (15462)
  (( segid "BrD " and resid 74   and name HB2 ))
  (  segid "BrD " and resid 74   and name HE% )
     3.600     3.200     1.900 peak 15482 weight  0.11000E+01 volume  0.37941E+02 ppm1      2.985 ppm2      7.533
ASSI (15492)
  (( segid "BrD " and resid 74   and name HB1 ))
  (  segid "BrD " and resid 74   and name HE% )
     2.800     2.000     2.000 peak 15492 weight  0.11000E+01 volume  0.16094E+03 ppm1      3.571 ppm2      7.535
ASSI (15602)
  (( segid "BrD " and resid 82   and name HB2 ))
  (  segid "BrD " and resid 82   and name HE% )
     3.000     2.200     2.200 peak 15602 weight  0.11000E+01 volume  0.11655E+03 ppm1      3.573 ppm2      7.069
ASSI (15612)
  (( segid "BrD " and resid 82   and name HB1 ))
  (  segid "BrD " and resid 82   and name HE% )
     2.800     2.000     2.000 peak 15612 weight  0.11000E+01 volume  0.15106E+03 ppm1      3.672 ppm2      7.069
ASSI (15732)
  (( segid "BrD " and resid 82   and name HA ))
  (  segid "BrD " and resid 82   and name HE% )
     3.200     2.600     2.300 peak 15732 weight  0.11000E+01 volume  0.68425E+02 ppm1      4.755 ppm2      7.063
ASSI (15742)
  (( segid "BrD " and resid 82   and name HA ))
  (  segid "BrD " and resid 82   and name HD% )
     2.100     1.100     1.100 peak 15742 weight  0.11000E+01 volume  0.82972E+03 ppm1      4.755 ppm2      7.259
ASSI (15792)
  (( segid "BrD " and resid 15   and name HA ))
  (  segid "BrD " and resid 18   and name HD2%)
     4.600     4.600     0.900 peak 15792 weight  0.11000E+01 volume  0.83712E+01 ppm1      4.607 ppm2      0.408
ASSI (16522)
  (( segid "BrD " and resid 107  and name HA ))
  (  segid "BrD " and resid 107  and name HE% )
     2.700     1.800     1.800 peak 16522 weight  0.11000E+01 volume  0.21131E+03 ppm1      4.410 ppm2      7.901
ASSI (16532)
  (( segid "BrD " and resid 96   and name HA ))
  (  segid "BrD " and resid 96   and name HE% )
     2.800     2.000     2.000 peak 16532 weight  0.11000E+01 volume  0.16900E+03 ppm1      4.410 ppm2      7.607
ASSI (16692)
  (( segid "BrD " and resid 52   and name HA ))
  (( segid "BrD " and resid 53   and name HG2 ))
     5.500     5.500     0.000 peak 16692 weight  0.11000E+01 volume  0.97221E+00 ppm1      5.592 ppm2      2.494
ASSI (16822)
  (( segid "BrD " and resid 105  and name HB1 ))
  (( segid "BrD " and resid 105  and name HA  ))
     2.600     1.700     1.700 peak 16822 weight  0.11000E+01 volume  0.25358E+03 ppm1      3.721 ppm2      4.932
ASSI (17182)
  (( segid "BrD " and resid 105  and name HB2 ))
  (( segid "BrD " and resid 105  and name HA  ))
     2.400     1.400     1.400 peak 17182 weight  0.11000E+01 volume  0.43854E+03 ppm1      3.668 ppm2      4.932
ASSI (17202)
  (( segid "BrD " and resid 105  and name HB2 ))
  (  segid "BrD " and resid 105  and name HD% )
     2.200     1.200     1.200 peak 17202 weight  0.11000E+01 volume  0.67242E+03 ppm1      3.720 ppm2      7.788
ASSI (17242)
  (( segid "BrD " and resid 105  and name HA  ))
  (  segid "BrD " and resid 105  and name HD% )
     2.200     1.200     1.200 peak 17242 weight  0.11000E+01 volume  0.69463E+03 ppm1      4.903 ppm2      7.787
ASSI (17292)
  (( segid "BrD " and resid 116  and name HA ))
  (( segid "BrD " and resid 116  and name HG12))
     2.800     2.000     2.000 peak 17292 weight  0.11000E+01 volume  0.16843E+03 ppm1      4.804 ppm2      1.554
ASSI (17302)
  (( segid "BrD " and resid 116  and name HA ))
  (( segid "BrD " and resid 116  and name HG11))
     3.100     2.400     2.400 peak 17302 weight  0.11000E+01 volume  0.94615E+02 ppm1      4.804 ppm2      1.917
ASSI (17412)
  (( segid "BrD " and resid 34   and name HB2 ))
  (  segid "BrD " and resid 34   and name HD% )
     2.900     2.100     2.100 peak 17412 weight  0.11000E+01 volume  0.12277E+03 ppm1      3.125 ppm2      7.705
ASSI (17652)
  (  segid "BrD " and resid 81   and name HG2%)
  (( segid "BrD " and resid 34   and name HA ))
     2.500     1.600     1.600 peak 17652 weight  0.11000E+01 volume  0.31158E+03 ppm1      0.760 ppm2      5.542
ASSI (17662)
  (  segid "BrD " and resid 81   and name HG2%)
  (( segid "BrD " and resid 55   and name HA ))
     2.600     1.700     1.700 peak 17662 weight  0.11000E+01 volume  0.23078E+03 ppm1      0.755 ppm2      5.366
ASSI (17722)
  (( segid "BrD " and resid 33   and name HG1 ))
  (( segid "BrD " and resid 33   and name HA ))
     3.100     2.400     2.400 peak 17722 weight  0.11000E+01 volume  0.93743E+02 ppm1      0.859 ppm2      4.354
ASSI (17812)
  (( segid "BrD " and resid 33   and name HD2 ))
  (( segid "BrD " and resid 33   and name HB2 ))
     3.000     2.200     2.200 peak 17812 weight  0.11000E+01 volume  0.10412E+03 ppm1      2.190 ppm2     -0.162
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ASSI (17822)
  (( segid "BrD " and resid 33   and name HD1 ))
  (( segid "BrD " and resid 33   and name HB2 ))
    3.000     2.200     2.200 peak 17822 weight  0.11000E+01 volume  0.99908E+02 ppm1     2.782 ppm2     -0.162
ASSI (17832)
  (( segid "BrD " and resid 33   and name HD2 ))
  (( segid "BrD " and resid 33   and name HA  ))
    3.900     3.800     1.600 peak 17832 weight  0.11000E+01 volume  0.24295E+02 ppm1     2.190 ppm2     4.354
ASSI (17842)
  (( segid "BrD " and resid 33   and name HD1 ))
  (( segid "BrD " and resid 33   and name HA  ))
    3.800     3.600     1.700 peak 17842 weight  0.11000E+01 volume  0.26770E+02 ppm1     2.785 ppm2     4.353
ASSI (17862)
  (( segid "BrD " and resid 33   and name HD2 ))
  (( segid "BrD " and resid 32   and name HA  ))
    3.300     2.700     2.200 peak 17862 weight  0.11000E+01 volume  0.62722E+02 ppm1     2.190 ppm2     4.981
ASSI (17872)
  (( segid "BrD " and resid 33   and name HD1 ))
  (( segid "BrD " and resid 32   and name HN2 ))
    5.500     5.500     0.000 peak 17872 weight  0.11000E+01 volume  0.61193E-03 ppm1     2.783 ppm2     7.797
ASSI (17882)
  (( segid "BrD " and resid 33   and name HD2 ))
  (( segid "BrD " and resid 32   and name HN2 ))
    5.500     5.500     0.000 peak 17882 weight  0.11000E+01 volume  0.56139E-03 ppm1     2.191 ppm2     7.797
ASSI (17912)
  (( segid "BrD " and resid 33   and name HB1 ))
  (( segid "BrD " and resid 33   and name HD2 ))
    3.900     3.800     1.600 peak 17912 weight  0.11000E+01 volume  0.21009E+02 ppm1     1.056 ppm2     2.190
ASSI (17942)
  (( segid "BrD " and resid 33   and name HB1 ))
  (( segid "BrD " and resid 33   and name HD1 ))
    3.300     2.700     2.200 peak 17942 weight  0.11000E+01 volume  0.67464E+02 ppm1     1.056 ppm2     2.792
ASSI (18062)
  (( segid "BrD " and resid 75   and name HG1 ))
  (  segid "BrD " and resid 110  and name HG2% )
    4.000     4.000     1.500 peak 18062 weight  0.11000E+01 volume  0.20766E+02 ppm1     3.522 ppm2     1.262
ASSI (18082)
  (( segid "BrD " and resid 75   and name HG2 ))
  (  segid "BrD " and resid 110  and name HD1% )
    3.400     2.900     2.100 peak 18082 weight  0.11000E+01 volume  0.48309E+02 ppm1     3.226 ppm2     1.140
ASSI (18092)
  (( segid "BrD " and resid 75   and name HG2 ))
  (  segid "BrD " and resid 110  and name HG2% )
    4.100     4.100     1.400 peak 18092 weight  0.11000E+01 volume  0.17226E+02 ppm1     3.226 ppm2     1.262
ASSI (18162)
  (( segid "BrD " and resid 53   and name HB1 ))
  (( segid "BrD " and resid 52   and name HA  ))
    5.500     5.500     0.000 peak 18162 weight  0.11000E+01 volume  0.54558E+00 ppm1     2.784 ppm2     5.582
ASSI (18172)
  (( segid "BrD " and resid 53   and name HB1 ))
  (  segid "BrD " and resid 46   and name HE% )
    2.600     1.700     1.700 peak 18172 weight  0.11000E+01 volume  0.27274E+03 ppm1     2.783 ppm2     6.688
ASSI (18182)
  (( segid "BrD " and resid 53   and name HB1 ))
  (  segid "BrD " and resid 47   and name HE% )
    2.500     1.600     1.600 peak 18182 weight  0.11000E+01 volume  0.34975E+03 ppm1     2.783 ppm2     7.267
ASSI (18192)
  (( segid "BrD " and resid 53   and name HA  ))
  (  segid "BrD " and resid 47   and name HD% )
    3.100     2.400     2.400 peak 18192 weight  0.11000E+01 volume  0.93621E+02 ppm1     2.777 ppm2     7.962
ASSI (18222)
  (  segid "BrD " and resid 35   and name HE% )
  (( segid "BrD " and resid 35   and name HG1 ))
    2.300     1.300     1.300 peak 18222 weight  0.11000E+01 volume  0.50180E+03 ppm1     2.781 ppm2     3.648
ASSI (18292)
  (  segid "BrD " and resid 35   and name HE% )
  (( segid "BrD " and resid 35   and name HA  ))
    2.700     1.800     1.800 peak 18292 weight  0.11000E+01 volume  0.21224E+03 ppm1     2.782 ppm2     4.901
ASSI (18452)
  (( segid "BrD " and resid 75   and name HG2 ))
  (  segid "BrD " and resid 74   and name HD% )
    3.400     2.900     2.100 peak 18452 weight  0.11000E+01 volume  0.49200E+02 ppm1     3.227 ppm2     6.999
ASSI (18462)
  (( segid "BrD " and resid 75   and name HG1 ))
  (  segid "BrD " and resid 74   and name HD% )
    3.100     2.400     2.400 peak 18462 weight  0.11000E+01 volume  0.92286E+02 ppm1     3.524 ppm2     7.001
ASSI (18512)
  (  segid "BrD " and resid 75   and name HE% )
  (( segid "BrD " and resid 75   and name HA  ))
    2.900     2.100     2.100 peak 18512 weight  0.11000E+01 volume  0.12672E+03 ppm1     2.635 ppm2     4.518
ASSI (18752)
  (  segid "BrD " and resid 75   and name HE% )
  (  segid "BrD " and resid 18   and name HD2% )
    3.800     3.600     1.700 peak 18752 weight  0.11000E+01 volume  0.27479E+02 ppm1     2.634 ppm2     0.416
ASSI (18792)
  (  segid "BrD " and resid 75   and name HE% )
  (  segid "BrD " and resid 110  and name HG2% )
    2.700     1.800     1.800 peak 18792 weight  0.11000E+01 volume  0.21856E+03 ppm1     2.634 ppm2     1.262
ASSI (18802)
  (  segid "BrD " and resid 75   and name HE% )
  (  segid "BrD " and resid 110  and name HD1% )
    2.600     1.700     1.700 peak 18802 weight  0.11000E+01 volume  0.24635E+03 ppm1     2.634 ppm2     1.140
ASSI (19032)
  (( segid "BrD " and resid 75   and name HA  ))
  (  segid "BrD " and resid 74   and name HD% )
    2.600     1.700     1.700 peak 19032 weight  0.11000E+01 volume  0.28302E+03 ppm1     4.508 ppm2     6.998
ASSI (19112)
  (  segid "BrD " and resid 42   and name HB% )
  (  segid "BrD " and resid 88   and name HE% )
    2.900     2.100     2.100 peak 19112 weight  0.11000E+01 volume  0.13802E+03 ppm1     1.700 ppm2     7.416
ASSI (19132)
  (  segid "BrD " and resid 43   and name HB% )
  (  segid "BrD " and resid 88   and name HD% )
    4.900     4.900     0.600 peak 19132 weight  0.11000E+01 volume  0.55156E+01 ppm1     1.697 ppm2     7.609
ASSI (19142)
  (  segid "BrD " and resid 43   and name HB% )
  (  segid "BrD " and resid 46   and name HE% )
    3.400     2.900     2.100 peak 19142 weight  0.11000E+01 volume  0.52712E+02 ppm1     1.697 ppm2     6.689
ASSI (19162)
  (  segid "BrD " and resid 43   and name HB% )
  (  segid "BrD " and resid 46   and name HD% )
    2.600     1.700     1.700 peak 19162 weight  0.11000E+01 volume  0.28846E+03 ppm1     1.697 ppm2     5.753
ASSI (19852)
  (( segid "BrD " and resid 102  and name HA  ))
  (( segid "BrD " and resid 102  and name HG  ))
    2.700     1.800     1.800 peak 19852 weight  0.11000E+01 volume  0.19930E+03 ppm1     4.263 ppm2     2.157
ASSI (20082)
  (( segid "BrD " and resid 110  and name HA  ))
  (( segid "BrD " and resid 110  and name HG11))
    2.400     1.400     1.400 peak 20082 weight  0.11000E+01 volume  0.38344E+03 ppm1     4.411 ppm2     1.718
ASSI (20232)
  (  segid "BrD " and resid 17   and name HG2%)
  (( segid "BrD " and resid 18   and name HA  ))
    3.100     2.400     2.400 peak 20232 weight  0.11000E+01 volume  0.91939E+02 ppm1     1.747 ppm2     3.882
ASSI (20342)
  (( segid "BrD " and resid 53   and name HA  ))
  (( segid "BrD " and resid 53   and name HD1 ))
    3.300     2.700     2.200 peak 20342 weight  0.11000E+01 volume  0.66608E+02 ppm1     4.696 ppm2     4.210
ASSI (20372)
  (( segid "BrD " and resid 53   and name HA  ))
  (  segid "BrD " and resid 47   and name HE% )
    3.900     3.800     1.600 peak 20372 weight  0.11000E+01 volume  0.22677E+02 ppm1     4.696 ppm2     7.260
ASSI (20422)
  (( segid "BrD " and resid 53   and name HD2 ))
  (( segid "BrD " and resid 53   and name HA  ))
    3.200     2.600     2.300 peak 20422 weight  0.11000E+01 volume  0.75265E+02 ppm1     4.015 ppm2     4.696
ASSI (20432)
  (( segid "BrD " and resid 53   and name HD1 ))
  (  segid "BrD " and resid 50   and name HG2%)
    3.400     2.900     2.100 peak 20432 weight  0.11000E+01 volume  0.50650E+02 ppm1     4.214 ppm2     0.993
ASSI (20462)
  (( segid "BrD " and resid 53   and name HG1 ))
  (  segid "BrD " and resid 46   and name HE% )
    3.600     3.200     1.900 peak 20462 weight  0.11000E+01 volume  0.35265E+02 ppm1     2.784 ppm2     6.689
ASSI (20472)
  (( segid "BrD " and resid 53   and name HG1 ))
  (  segid "BrD " and resid 47   and name HE% )
    2.500     1.600     1.600 peak 20472 weight  0.11000E+01 volume  0.29199E+03 ppm1     2.784 ppm2     7.267
ASSI (20482)
  (( segid "BrD " and resid 53   and name HG2 ))
  (  segid "BrD " and resid 47   and name HE% )
    2.600     1.700     1.700 peak 20482 weight  0.11000E+01 volume  0.27122E+03 ppm1     2.486 ppm2     7.267
ASSI (20492)
  (( segid "BrD " and resid 53   and name HG2 ))
  (  segid "BrD " and resid 47   and name HD% )
    2.400     1.400     1.400 peak 20492 weight  0.11000E+01 volume  0.38647E+03 ppm1     2.486 ppm2     7.958
ASSI (20502)
  (( segid "BrD " and resid 53   and name HG1 ))
  (  segid "BrD " and resid 47   and name HD% )
    2.800     2.000     2.000 peak 20502 weight  0.11000E+01 volume  0.16213E+03 ppm1     2.784 ppm2     7.958
ASSI (20522)
  (( segid "BrD " and resid 53   and name HG1 ))
  (( segid "BrD " and resid 52   and name HA  ))
    5.500     5.500     0.000 peak 20522 weight  0.11000E+01 volume  0.58337E-01 ppm1     2.784 ppm2     5.587
ASSI (20602)
  (( segid "BrD " and resid 61   and name HG2 ))
  (( segid "BrD " and resid 58   and name HA  ))
    2.500     1.600     1.600 peak 20602 weight  0.11000E+01 volume  0.31153E+03 ppm1     2.831 ppm2     4.452
ASSI (20612)
  (( segid "BrD " and resid 61   and name HG1 ))
  (( segid "BrD " and resid 58   and name HA  ))
    2.500     1.600     1.600 peak 20612 weight  0.11000E+01 volume  0.36307E+03 ppm1     2.980 ppm2     4.452
ASSI (20702)
  (( segid "BrD " and resid 80   and name HA  ))
  (( segid "BrD " and resid 83   and name HB  ))
    1.400     0.500     0.800 peak 20702 weight  0.11000E+01 volume  0.11465E+05 ppm1     4.656 ppm2     4.804
ASSI (20772)
  (( segid "BrD " and resid 58   and name HB  ))
  (( segid "BrD " and resid 54   and name HA  ))
    3.400     2.900     2.100 peak 20772 weight  0.11000E+01 volume  0.51113E+02 ppm1     4.702 ppm2     5.544
ASSI (20782)
  (  segid "BrD " and resid 58   and name HG2%)
  (( segid "BrD " and resid 54   and name HA  ))
    2.800     2.000     2.000 peak 20782 weight  0.11000E+01 volume  0.15234E+03 ppm1     1.648 ppm2     5.542
ASSI (20882)
  (( segid "BrD " and resid 62   and name HD1 ))
  (( segid "BrD " and resid 62   and name HA  ))
    3.100     2.400     2.400 peak 20882 weight  0.11000E+01 volume  0.94082E+02 ppm1     3.177 ppm2     4.476
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ASSI (20892)
  (( segid "BrD " and resid 62   and name HD2 ))
  (( segid "BrD " and resid 62   and name HA  ))
     3.000     2.200     2.200 peak 20892 weight  0.11000E+01 volume  0.10111E+03 ppm1      2.634 ppm2      4.476
ASSI (20902)
  (( segid "BrD " and resid 62   and name HD1 ))
  (  segid "BrD " and resid 67   and name HE% )
     4.400     4.400     1.100 peak 20902 weight  0.11000E+01 volume  0.11575E+02 ppm1      3.177 ppm2      7.316
ASSI (20912)
  (( segid "BrD " and resid 62   and name HD1 ))
  (  segid "BrD " and resid 67   and name HD% )
     3.700     3.400     1.800 peak 20912 weight  0.11000E+01 volume  0.30541E+02 ppm1      3.177 ppm2      6.893
ASSI (20922)
  (( segid "BrD " and resid 62   and name HD2 ))
  (  segid "BrD " and resid 67   and name HD% )
     3.400     2.900     2.100 peak 20922 weight  0.11000E+01 volume  0.54284E+02 ppm1      2.634 ppm2      6.893
ASSI (20932)
  (( segid "BrD " and resid 62   and name HD2 ))
  (  segid "BrD " and resid 67   and name HE% )
     3.100     2.400     2.400 peak 20932 weight  0.11000E+01 volume  0.91289E+02 ppm1      2.634 ppm2      7.315
ASSI (20952)
  (( segid "BrD " and resid 62   and name HB1 ))
  (( segid "BrD " and resid 62   and name HD1 ))
     2.200     2.600     2.300 peak 20952 weight  0.11000E+01 volume  0.71708E+02 ppm1      2.641 ppm2      3.183
ASSI (20962)
  (( segid "BrD " and resid 62   and name HB2 ))
  (( segid "BrD " and resid 62   and name HG1 ))
     3.000     2.200     2.200 peak 20962 weight  0.11000E+01 volume  0.10075E+03 ppm1      1.699 ppm2      2.325
ASSI (20972)
  (( segid "BrD " and resid 62   and name HG2 ))
  (( segid "BrD " and resid 62   and name HB1 ))
     2.700     1.800     1.800 peak 20972 weight  0.11000E+01 volume  0.20830E+03 ppm1      2.641 ppm2      1.479
ASSI (21012)
  (( segid "BrD " and resid 62   and name HG2 ))
  (( segid "BrD " and resid 62   and name HD1 ))
     3.100     2.400     2.400 peak 21012 weight  0.11000E+01 volume  0.87215E+02 ppm1      1.501 ppm2      3.182
ASSI (21022)
  (( segid "BrD " and resid 62   and name HG1 ))
  (( segid "BrD " and resid 62   and name HA  ))
     2.900     2.100     2.100 peak 21022 weight  0.11000E+01 volume  0.13858E+03 ppm1      2.340 ppm2      4.474
ASSI (21162)
  (( segid "BrD " and resid 83   and name HA  ))
  (( segid "BrD " and resid 86   and name HG2 ))
     4.800     4.800     0.700 peak 21162 weight  0.11000E+01 volume  0.66244E+01 ppm1      4.459 ppm2      0.766
ASSI (21512)
  (( segid "BrD " and resid 38   and name HB  ))
  (  segid "BrD " and resid 46   and name HD% )
     3.400     2.900     2.100 peak 21512 weight  0.11000E+01 volume  0.54169E+02 ppm1      1.747 ppm2      5.745
ASSI (21522)
  (( segid "BrD " and resid 38   and name HB  ))
  (  segid "BrD " and resid 47   and name HE% )
     4.500     4.500     1.000 peak 21522 weight  0.11000E+01 volume  0.90841E+01 ppm1      1.751 ppm2      7.259
ASSI (21532)
  (( segid "BrD " and resid 38   and name HB  ))
  (  segid "BrD " and resid 46   and name HE% )
     4.500     4.500     1.000 peak 21532 weight  0.11000E+01 volume  0.97356E+01 ppm1      1.747 ppm2      6.689
ASSI (21602)
  (  segid "BrD " and resid 81   and name HG1% )
  (( segid "BrD " and resid 34   and name HB2 ))
     3.300     2.700     2.200 peak 21602 weight  0.11000E+01 volume  0.56657E+02 ppm1      1.056 ppm2      3.146
ASSI (21622)
  (  segid "BrD " and resid 81   and name HG1% )
  (( segid "BrD " and resid 55   and name HA  ))
     2.400     1.400     1.400 peak 21622 weight  0.11000E+01 volume  0.44267E+03 ppm1      1.056 ppm2      5.367
ASSI (21632)
  (  segid "BrD " and resid 81   and name HG1% )
  (( segid "BrD " and resid 34   and name HA  ))
     2.800     2.000     2.000 peak 21632 weight  0.11000E+01 volume  0.15411E+03 ppm1      1.056 ppm2      5.542
ASSI (21762)
  (  segid "BrD " and resid 81   and name HG2% )
  (( segid "BrD " and resid 78   and name HA  ))
     2.600     1.700     1.700 peak 21762 weight  0.11000E+01 volume  0.24983E+03 ppm1      0.760 ppm2      4.004
ASSI (21832)
  (  segid "BrD " and resid 50   and name HD1% )
  (  segid "BrD " and resid 49   and name HG1% )
     2.900     2.100     2.100 peak 21832 weight  0.11000E+01 volume  0.14668E+03 ppm1      1.155 ppm2      1.645
ASSI (21842)
  (  segid "BrD " and resid 50   and name HD1% )
  (  segid "BrD " and resid 49   and name HG2% )
     2.400     1.400     1.400 peak 21842 weight  0.11000E+01 volume  0.37404E+03 ppm1      1.155 ppm2      1.571
ASSI (21852)
  (( segid "BrD " and resid 49   and name HB  ))
  (  segid "BrD " and resid 88   and name HD% )
     3.400     2.900     2.100 peak 21852 weight  0.11000E+01 volume  0.48521E+02 ppm1      2.634 ppm2      7.606
ASSI (21862)
  (( segid "BrD " and resid 49   and name HB  ))
  (  segid "BrD " and resid 88   and name HE% )
     3.400     2.900     2.100 peak 21862 weight  0.11000E+01 volume  0.55049E+02 ppm1      2.634 ppm2      7.414
ASSI (21872)
  (( segid "BrD " and resid 49   and name HB  ))
  (( segid "BrD " and resid 46   and name HA  ))
     3.700     3.400     1.800 peak 21872 weight  0.11000E+01 volume  0.31537E+03 ppm1      2.634 ppm2      4.163
ASSI (21912)
  (  segid "BrD " and resid 50   and name HD1% )
  (( segid "BrD " and resid 87   and name HB2 ))
     2.600     1.700     1.700 peak 21912 weight  0.11000E+01 volume  0.24085E+03 ppm1      1.155 ppm2      2.603
ASSI (21932)
  (  segid "BrD " and resid 50   and name HD1% )
  (( segid "BrD " and resid 87   and name HB1 ))
     2.400     1.400     1.400 peak 21932 weight  0.11000E+01 volume  0.36901E+03 ppm1      1.155 ppm2      2.778
ASSI (21932)
  (  segid "BrD " and resid 50   and name HD1% )
  (( segid "BrD " and resid 87   and name HG1 ))
     3.700     3.400     1.800 peak 21932 weight  0.11000E+01 volume  0.32396E+02 ppm1      1.155 ppm2      3.028
ASSI (21942)
  (  segid "BrD " and resid 50   and name HD1% )
  (( segid "BrD " and resid 84   and name HB2 ))
     2.700     1.800     1.800 peak 21942 weight  0.11000E+01 volume  0.22842E+03 ppm1      1.155 ppm2      3.272
ASSI (21962)
  (  segid "BrD " and resid 50   and name HD1% )
  (( segid "BrD " and resid 84   and name HB1 ))
     2.600     1.700     1.700 peak 21962 weight  0.11000E+01 volume  0.28478E+03 ppm1      1.155 ppm2      3.606
ASSI (21992)
  (  segid "BrD " and resid 50   and name HD1% )
  (( segid "BrD " and resid 88   and name HA  ))
     2.700     1.800     1.800 peak 21992 weight  0.11000E+01 volume  0.19153E+03 ppm1      1.155 ppm2      4.988
ASSI (22002)
  (  segid "BrD " and resid 50   and name HD1% )
  (( segid "BrD " and resid 84   and name HA  ))
     2.300     1.300     1.300 peak 22002 weight  0.11000E+01 volume  0.57384E+03 ppm1      1.155 ppm2      4.915
ASSI (22052)
  (( segid "BrD " and resid 50   and name HB  ))
  (  segid "BrD " and resid 46   and name HE% )
     3.000     2.200     2.200 peak 22052 weight  0.11000E+01 volume  0.99146E+02 ppm1      1.797 ppm2      6.689
ASSI (22092)
  (  segid "BrD " and resid 50   and name HG2% )
  (( segid "BrD " and resid 52   and name HA  ))
     3.500     3.100     2.000 peak 22092 weight  0.11000E+01 volume  0.46395E+02 ppm1      1.006 ppm2      5.587
ASSI (22102)
  (  segid "BrD " and resid 50   and name HG2% )
  (  segid "BrD " and resid 46   and name HD% )
     3.700     3.400     1.800 peak 22102 weight  0.11000E+01 volume  0.30083E+02 ppm1      1.007 ppm2      5.745
ASSI (22152)
  (  segid "BrD " and resid 50   and name HG2% )
  (  segid "BrD " and resid 47   and name HE% )
     4.300     4.300     1.200 peak 22152 weight  0.11000E+01 volume  0.12530E+02 ppm1      1.007 ppm2      7.259
ASSI (22162)
  (  segid "BrD " and resid 50   and name HG2% )
  (  segid "BrD " and resid 46   and name HE% )
     2.500     1.600     1.600 peak 22162 weight  0.11000E+01 volume  0.31318E+03 ppm1      1.007 ppm2      6.689
ASSI (22172)
  (  segid "BrD " and resid 50   and name HG2% )
  (( segid "BrD " and resid 84   and name HA  ))
     2.900     2.100     2.100 peak 22172 weight  0.11000E+01 volume  0.14754E+03 ppm1      1.007 ppm2      4.915
ASSI (22192)
  (  segid "BrD " and resid 50   and name HG2% )
  (  segid "BrD " and resid 49   and name HG2% )
     3.700     3.400     1.800 peak 22192 weight  0.11000E+01 volume  0.30274E+02 ppm1      1.006 ppm2      1.570
ASSI (22262)
  (( segid "BrD " and resid 50   and name HG12 ))
  (( segid "BrD " and resid 50   and name HA  ))
     3.300     2.700     2.200 peak 22262 weight  0.11000E+01 volume  0.57888E+02 ppm1      0.809 ppm2      4.522
ASSI (22342)
  (  segid "BrD " and resid 69   and name HG2% )
  (( segid "BrD " and resid 70   and name HA  ))
     3.500     3.100     2.000 peak 22342 weight  0.11000E+01 volume  0.43395E+02 ppm1      1.427 ppm2      5.356
ASSI (22512)
  (  segid "BrD " and resid 49   and name HG1% )
  (  segid "BrD " and resid 88   and name HE% )
     2.300     1.300     1.300 peak 22512 weight  0.11000E+01 volume  0.52744E+03 ppm1      1.646 ppm2      7.419
ASSI (22522)
  (  segid "BrD " and resid 49   and name HG1% )
  (  segid "BrD " and resid 88   and name HD% )
     2.500     1.600     1.600 peak 22522 weight  0.11000E+01 volume  0.29406E+03 ppm1      1.646 ppm2      7.604
ASSI (22652)
  (( segid "BrD " and resid 7    and name HG1 ))
  (( segid "BrD " and resid 7    and name HA  ))
     3.000     2.200     2.200 peak 22652 weight  0.11000E+01 volume  0.11329E+03 ppm1      2.880 ppm2      5.143
ASSI (22792)
  (( segid "BrD " and resid 104  and name HB1 ))
  (( segid "BrD " and resid 101  and name HA  ))
     2.300     1.300     1.300 peak 22792 weight  0.11000E+01 volume  0.53108E+03 ppm1      2.537 ppm2      4.267
ASSI (22872)
  (( segid "BrD " and resid 6    and name HE1 ))
  (( segid "BrD " and resid 6    and name HA  ))
     2.100     1.100     1.100 peak 22872 weight  0.11000E+01 volume  0.98321E+03 ppm1      1.610 ppm2      4.972
ASSI (22942)
  (( segid "BrD " and resid 44   and name HD2 ))
  (( segid "BrD " and resid 44   and name HA  ))
     3.100     2.400     2.400 peak 22942 weight  0.11000E+01 volume  0.83098E+02 ppm1      4.114 ppm2      5.114
ASSI (23162)
  (( segid "BrD " and resid 8    and name HG1 ))
  (( segid "BrD " and resid 8    and name HA  ))
     2.600     1.700     1.700 peak 23162 weight  0.11000E+01 volume  0.28012E+03 ppm1      2.635 ppm2      5.021
ASSI (23172)
  (( segid "BrD " and resid 11   and name HG1 ))
  (( segid "BrD " and resid 10   and name HA  ))
     4.100     4.100     1.400 peak 23172 weight  0.11000E+01 volume  0.17156E+02 ppm1      2.635 ppm2      5.477
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ASSI (23302)
  (( segid "BrD " and resid 9    and name HD1 ))
  (( segid "BrD " and resid 9    and name HA  ))
    2.900     2.100     2.100 peak 23302 weight  0.11000E+01 volume  0.13154E+03 ppm1    3.768 ppm2    4.940
ASSI (23352)
  (( segid "BrD " and resid 9    and name HD1 ))
  (( segid "BrD " and resid 9    and name HB1 ))
    2.400     1.400     1.400 peak 23352 weight  0.11000E+01 volume  0.39945E+03 ppm1    3.768 ppm2    2.434
ASSI (23362)
  (( segid "BrD " and resid 9    and name HD1 ))
  (( segid "BrD " and resid 9    and name HB2 ))
    2.300     1.300     1.300 peak 23362 weight  0.11000E+01 volume  0.50335E+03 ppm1    3.768 ppm2    2.385
ASSI (23542)
  (( segid "BrD " and resid 11   and name HA  ))
  (( segid "BrD " and resid 11   and name HD1 ))
    2.600     1.700     1.700 peak 23542 weight  0.11000E+01 volume  0.23295E+03 ppm1    4.951 ppm2    4.459
ASSI (23552)
  (  segid "BrD " and resid 14   and name HD2%)
  (( segid "BrD " and resid 11   and name HA  ))
    2.500     1.600     1.600 peak 23552 weight  0.11000E+01 volume  0.34571E+03 ppm1    1.401 ppm2    4.947
ASSI (23692)
  (( segid "BrD " and resid 14   and name HB2 ))
  (  segid "BrD " and resid 18   and name HD1%)
    2.900     2.100     2.100 peak 23692 weight  0.11000E+01 volume  0.14113E+03 ppm1    2.143 ppm2    1.084
ASSI (23702)
  (( segid "BrD " and resid 14   and name HA  ))
  (  segid "BrD " and resid 17   and name HD2%)
    3.400     2.900     2.100 peak 23702 weight  0.11000E+01 volume  0.49626E+02 ppm1    4.656 ppm2    1.750
ASSI (23722)
  (( segid "BrD " and resid 14   and name HG  ))
  (  segid "BrD " and resid 18   and name HD2%)
    3.200     2.600     2.300 peak 23722 weight  0.11000E+01 volume  0.69871E+02 ppm1    2.044 ppm2    0.415
ASSI (23752)
  (( segid "BrD " and resid 14   and name HA  ))
  (( segid "BrD " and resid 17   and name HB  ))
    2.100     1.100     1.100 peak 23752 weight  0.11000E+01 volume  0.89711E+03 ppm1    4.656 ppm2    4.854
ASSI (23852)
  (  segid "BrD " and resid 14   and name HD1%)
  (( segid "BrD " and resid 11   and name HA  ))
    2.200     1.200     1.200 peak 23852 weight  0.11000E+01 volume  0.75160E+03 ppm1    1.402 ppm2    4.947
ASSI (23952)
  (( segid "BrD " and resid 18   and name HB2 ))
  (( segid "BrD " and resid 15   and name HA  ))
    3.200     2.600     2.300 peak 23952 weight  0.11000E+01 volume  0.79651E+02 ppm1    0.911 ppm2    4.630
ASSI (23962)
  (( segid "BrD " and resid 18   and name HB1 ))
  (( segid "BrD " and resid 15   and name HA  ))
    3.100     2.400     2.400 peak 23962 weight  0.11000E+01 volume  0.98332E+02 ppm1    2.144 ppm2    4.626
ASSI (24042)
  (  segid "BrD " and resid 18   and name HD2%)
  (( segid "BrD " and resid 17   and name HB  ))
    2.900     2.100     2.100 peak 24042 weight  0.11000E+01 volume  0.13399E+03 ppm1    0.414 ppm2    4.860
ASSI (24052)
  (  segid "BrD " and resid 18   and name HD2%)
  (  segid "BrD " and resid 74   and name HD% )
    2.500     1.600     1.600 peak 24052 weight  0.11000E+01 volume  0.29789E+03 ppm1    0.415 ppm2    6.998
ASSI (24062)
  (  segid "BrD " and resid 18   and name HD2%)
  (  segid "BrD " and resid 74   and name HE% )
    2.700     1.800     1.800 peak 24062 weight  0.11000E+01 volume  0.22219E+03 ppm1    0.415 ppm2    7.534
ASSI (24072)
  (  segid "BrD " and resid 18   and name HD2%)
  (( segid "BrD " and resid 74   and name HB1 ))
    3.200     2.600     2.300 peak 24072 weight  0.11000E+01 volume  0.70185E+02 ppm1    0.419 ppm2    3.565
ASSI (24082)
  (  segid "BrD " and resid 18   and name HD2%)
  (( segid "BrD " and resid 74   and name HB2 ))
    2.900     2.100     2.100 peak 24082 weight  0.11000E+01 volume  0.13658E+03 ppm1    0.415 ppm2    2.995
ASSI (24092)
  (  segid "BrD " and resid 18   and name HD2%)
  (  segid "BrD " and resid 63   and name HD1%)
    3.200     2.600     2.300 peak 24092 weight  0.11000E+01 volume  0.72578E+02 ppm1    0.414 ppm2    1.648
ASSI (24132)
  (  segid "BrD " and resid 18   and name HD2%)
  (( segid "BrD " and resid 74   and name HA  ))
    3.400     2.900     2.100 peak 24132 weight  0.11000E+01 volume  0.52592E+02 ppm1    0.414 ppm2    4.378
ASSI (24162)
  (  segid "BrD " and resid 18   and name HD1%)
  (  segid "BrD " and resid 74   and name HE% )
    3.000     2.200     2.200 peak 24162 weight  0.11000E+01 volume  0.10145E+03 ppm1    1.058 ppm2    7.536
ASSI (24182)
  (  segid "BrD " and resid 18   and name HD1%)
  (  segid "BrD " and resid 74   and name HD% )
    2.600     1.700     1.700 peak 24182 weight  0.11000E+01 volume  0.27877E+03 ppm1    1.056 ppm2    6.998
ASSI (24212)
  (  segid "BrD " and resid 18   and name HD1%)
  (( segid "BrD " and resid 74   and name HA  ))
    3.200     2.600     2.300 peak 24212 weight  0.11000E+01 volume  0.78587E+02 ppm1    1.056 ppm2    4.378
ASSI (24522)
  (  segid "BrD " and resid 63   and name HD1%)
  (( segid "BrD " and resid 19   and name HA  ))
    2.600     1.700     1.700 peak 24522 weight  0.11000E+01 volume  0.26998E+03 ppm1    1.647 ppm2    4.397
ASSI (24662)
  (  segid "BrD " and resid 63   and name HD2%)
  (  segid "BrD " and resid 18   and name HD1%)
    2.700     1.800     1.800 peak 24662 weight  0.11000E+01 volume  0.19359E+03 ppm1    1.498 ppm2    1.090
ASSI (24672)
  (  segid "BrD " and resid 63   and name HD2%)
  (( segid "BrD " and resid 18   and name HB2 ))
    5.500     5.500     0.000 peak 24672 weight  0.11000E+01 volume  0.20841E+01 ppm1    1.498 ppm2    0.928
ASSI (24742)
  (( segid "BrD " and resid 19   and name HB2 ))
  (( segid "BrD " and resid 19   and name HE1 ))
    4.000     4.000     1.500 peak 24742 weight  0.11000E+01 volume  0.20066E+02 ppm1    1.989 ppm2    3.525
ASSI (24752)
  (( segid "BrD " and resid 19   and name HB1 ))
  (( segid "BrD " and resid 19   and name HE1 ))
    3.300     2.700     2.200 peak 24752 weight  0.11000E+01 volume  0.65557E+02 ppm1    2.290 ppm2    3.525
ASSI (24762)
  (( segid "BrD " and resid 19   and name HG1 ))
  (( segid "BrD " and resid 16   and name HA  ))
    2.900     2.100     2.100 peak 24762 weight  0.11000E+01 volume  0.12763E+03 ppm1    1.894 ppm2    4.508
ASSI (24812)
  (( segid "BrD " and resid 19   and name HD1 ))
  (( segid "BrD " and resid 16   and name HA  ))
    2.300     1.300     1.300 peak 24812 weight  0.11000E+01 volume  0.50116E+03 ppm1    2.192 ppm2    4.507
ASSI (24872)
  (( segid "BrD " and resid 23   and name HG1 ))
  (( segid "BrD " and resid 20   and name HA  ))
    3.100     2.400     2.400 peak 24872 weight  0.11000E+01 volume  0.91712E+02 ppm1    3.124 ppm2    4.893
ASSI (24902)
  (( segid "BrD " and resid 24   and name HG1 ))
  (( segid "BrD " and resid 21   and name HA  ))
    3.200     2.600     2.300 peak 24902 weight  0.11000E+01 volume  0.67606E+02 ppm1    3.469 ppm2    4.370
ASSI (24912)
  (( segid "BrD " and resid 24   and name HG2 ))
  (( segid "BrD " and resid 21   and name HA  ))
    2.600     1.700     1.700 peak 24912 weight  0.11000E+01 volume  0.26410E+03 ppm1    3.076 ppm2    4.370
ASSI (24932)
  (( segid "BrD " and resid 24   and name HA  ))
  (( segid "BrD " and resid 24   and name HB1 ))
    2.300     1.200     1.200 peak 24932 weight  0.11000E+01 volume  0.62910E+03 ppm1    4.784 ppm2    3.074
ASSI (25432)
  (( segid "BrD " and resid 85   and name HB1 ))
  (( segid "BrD " and resid 82   and name HA  ))
    3.100     2.400     2.400 peak 25432 weight  0.11000E+01 volume  0.87929E+02 ppm1    3.917 ppm2    4.753
ASSI (25552)
  (( segid "BrD " and resid 101  and name HG12))
  (( segid "BrD " and resid 101  and name HB  ))
    2.300     1.300     1.300 peak 25552 weight  0.11000E+01 volume  0.55437E+03 ppm1    1.797 ppm2    2.538
ASSI (25612)
  (  segid "BrD " and resid 21   and name HG2%)
  (( segid "BrD " and resid 18   and name HA  ))
    1.000     2.200     2.200 peak 25612 weight  0.11000E+01 volume  0.11167E+03 ppm1    1.599 ppm2    3.890
ASSI (26032)
  (  segid "BrD " and resid 110  and name HD1%)
  (( segid "BrD " and resid 75   and name HG1 ))
    3.400     2.900     2.100 peak 26032 weight  0.11000E+01 volume  0.51048E+02 ppm1    1.155 ppm2    3.524
ASSI (26172)
  (  segid "BrD " and resid 110  and name HG2%)
  (  segid "BrD " and resid 18   and name HD2%)
    4.400     4.400     1.100 peak 26172 weight  0.11000E+01 volume  0.11733E+02 ppm1    1.254 ppm2    0.408
ASSI (26182)
  (  segid "BrD " and resid 110  and name HD1%)
  (  segid "BrD " and resid 18   and name HD2%)
    3.000     2.200     2.200 peak 26182 weight  0.11000E+01 volume  0.11735E+03 ppm1    1.153 ppm2    0.410
ASSI (26302)
  (  segid "BrD " and resid 116  and name HD1%)
  (( segid "BrD " and resid 116  and name HA  ))
    2.500     1.600     1.600 peak 26302 weight  0.11000E+01 volume  0.31414E+03 ppm1    1.401 ppm2    4.826
ASSI (26562)
  (( segid "BrD " and resid 103  and name HA  ))
  (  segid "BrD " and resid 106  and name HD% )
    3.100     2.400     2.400 peak 26562 weight  0.11000E+01 volume  0.97052E+02 ppm1    3.768 ppm2    7.514
ASSI (26592)
  (( segid "BrD " and resid 103  and name HB1 ))
  (( segid "BrD " and resid 100  and name HA  ))
    2.700     1.800     1.800 peak 26592 weight  0.11000E+01 volume  0.20226E+03 ppm1    2.338 ppm2    4.946
ASSI (26642)
  (( segid "BrD " and resid 103  and name HB2 ))
  (( segid "BrD " and resid 103  and name HG2 ))
    2.000     1.000     1.000 peak 26642 weight  0.11000E+01 volume  0.14101E+04 ppm1    1.893 ppm2    2.520
ASSI (26652)
  (( segid "BrD " and resid 103  and name HB2 ))
  (( segid "BrD " and resid 103  and name HG1 ))
    2.200     1.200     1.200 peak 26652 weight  0.11000E+01 volume  0.62174E+03 ppm1    1.893 ppm2    2.598
ASSI (26662)
  (( segid "BrD " and resid 103  and name HG2 ))
  (( segid "BrD " and resid 100  and name HA  ))
    3.500     3.100     2.000 peak 26662 weight  0.11000E+01 volume  0.45243E+02 ppm1    2.519 ppm2    4.947
ASSI (26672)
  (( segid "BrD " and resid 103  and name HG1 ))
  (( segid "BrD " and resid 100  and name HA  ))
    3.900     3.800     1.600 peak 26672 weight  0.11000E+01 volume  0.23440E+02 ppm1    2.598 ppm2    4.947
ASSI (26722)
  (( segid "BrD " and resid 94   and name HG1 ))
  (( segid "BrD " and resid 32   and name HH2 ))
    2.900     2.100     2.100 peak 26722 weight  0.11000E+01 volume  0.14855E+03 ppm1    3.129 ppm2    7.788
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ASSI (26782)
  (( segid "BrD " and resid 94   and name HB1 ))
  (( segid "BrD " and resid 32   and name HZ2 ))
    2.500     1.600     1.600 peak 26782 weight  0.11000E+01 volume  0.35936E+03 ppm1     2.735 ppm2     7.998
ASSI (26793)
  (( segid "BrD " and resid 94   and name HB1 ))
  (( segid "BrD " and resid 32   and name HH2 ))
    3.000     2.200     2.200 peak 26792 weight  0.11000E+01 volume  0.10089E+03 ppm1     2.733 ppm2     7.785
ASSI (26842)
  (( segid "BrD " and resid 94   and name HG1 ))
  (( segid "BrD " and resid 94   and name HB1 ))
    2.200     1.200     1.200 peak 26842 weight  0.11000E+01 volume  0.72639E+03 ppm1     3.123 ppm2     2.731
ASSI (26862)
  (( segid "BrD " and resid 87   and name HG2 ))
  (( segid "BrD " and resid 86   and name HD1 ))
    3.600     3.200     1.900 peak 26862 weight  0.11000E+01 volume  0.34874E+02 ppm1     2.782 ppm2     1.900
ASSI (26882)
  (( segid "BrD " and resid 87   and name HB1 ))
  (( segid "BrD " and resid 87   and name HG1 ))
    2.400     1.400     1.400 peak 26882 weight  0.11000E+01 volume  0.47090E+03 ppm1     2.779 ppm2     3.021
ASSI (27152)
  (( segid "BrD " and resid 80   and name HD2 ))
  (( segid "BrD " and resid 80   and name HA  ))
    2.400     1.400     1.400 peak 27152 weight  0.11000E+01 volume  0.41973E+03 ppm1     3.912 ppm2     4.678
ASSI (27162)
  (( segid "BrD " and resid 80   and name HD1 ))
  (( segid "BrD " and resid 80   and name HA  ))
    2.600     1.700     1.700 peak 27162 weight  0.11000E+01 volume  0.27730E+03 ppm1     3.962 ppm2     4.677
ASSI (27212)
  (( segid "BrD " and resid 77   and name HB1 ))
  (( segid "BrD " and resid 74   and name HA  ))
    2.800     2.000     2.000 peak 27212 weight  0.11000E+01 volume  0.16302E+03 ppm1     3.325 ppm2     4.378
ASSI (27242)
  (( segid "BrD " and resid 80   and name HB2 ))
  (( segid "BrD " and resid 80   and name HD1 ))
    2.900     2.100     2.100 peak 27242 weight  0.11000E+01 volume  0.12614E+03 ppm1     2.536 ppm2     3.955
ASSI (27252)
  (( segid "BrD " and resid 80   and name HB2 ))
  (( segid "BrD " and resid 80   and name HD2 ))
    2.800     2.000     2.000 peak 27252 weight  0.11000E+01 volume  0.14981E+03 ppm1     2.536 ppm2     3.890
ASSI (27312)
  (( segid "BrD " and resid 56   and name HG  ))
  (( segid "BrD " and resid 34   and name HA  ))
    5.500     5.500     0.000 peak 27312 weight  0.11000E+01 volume  0.47841E+00 ppm1     2.338 ppm2     5.542
ASSI (27352)
  (( segid "BrD " and resid 55   and name HB1 ))
  (( segid "BrD " and resid 55   and name HA  ))
    2.200     1.200     1.200 peak 27352 weight  0.11000E+01 volume  0.72273E+03 ppm1     2.979 ppm2     5.366
ASSI (27412)
  (  segid "BrD " and resid 81   and name HG1%)
  (( segid "BrD " and resid 34   and name HB1 ))
    3.100     2.400     2.400 peak 27412 weight  0.11000E+01 volume  0.93003E+02 ppm1     1.058 ppm2     4.106
ASSI (27512)
  (  segid "BrD " and resid 22   and name HD2%)
  (( segid "BrD " and resid 22   and name HG  ))
    1.900     0.900     0.900 peak 27512 weight  0.11000E+01 volume  0.14735E+04 ppm1     1.599 ppm2     2.362
ASSI (27522)
  (  segid "BrD " and resid 22   and name HD2%)
  (( segid "BrD " and resid 22   and name HB2 ))
    2.200     1.200     1.200 peak 27522 weight  0.11000E+01 volume  0.70123E+03 ppm1     1.599 ppm2     2.286
ASSI (27682)
  (  segid "BrD " and resid 73   and name HD2%)
  (( segid "BrD " and resid 73   and name HB2 ))
    2.900     2.100     2.100 peak 27682 weight  0.11000E+01 volume  0.12667E+03 ppm1     1.600 ppm2     2.483
ASSI (27922)
  (  segid "BrD " and resid 78   and name HD1%)
  (  segid "BrD " and resid 82   and name HD% )
    3.600     3.200     1.900 peak 27922 weight  0.11000E+01 volume  0.39776E+02 ppm1     0.760 ppm2     7.259
ASSI (27972)
  (  segid "BrD " and resid 78   and name HD2%)
  (  segid "BrD " and resid 82   and name HD% )
    3.400     2.900     2.100 peak 27972 weight  0.11000E+01 volume  0.49710E+02 ppm1     0.662 ppm2     7.259
ASSI (28242)
  (  segid "BrD " and resid 56   and name HD1%)
  (( segid "BrD " and resid 34   and name HB1 ))
    3.000     2.200     2.200 peak 28242 weight  0.11000E+01 volume  0.10505E+03 ppm1     1.549 ppm2     4.110
ASSI (28282)
  (  segid "BrD " and resid 56   and name HD2%)
  (( segid "BrD " and resid 34   and name HA  ))
    3.800     3.600     1.700 peak 28282 weight  0.11000E+01 volume  0.25930E+02 ppm1     1.253 ppm2     5.540
ASSI (28312)
  (  segid "BrD " and resid 56   and name HD2%)
  (( segid "BrD " and resid 34   and name HB1 ))
    3.400     2.900     2.100 peak 28312 weight  0.11000E+01 volume  0.48455E+02 ppm1     1.253 ppm2     4.110
ASSI (28362)
  (  segid "BrD " and resid 56   and name HD2%)
  (( segid "BrD " and resid 34   and name HB2 ))
    3.200     2.600     2.300 peak 28362 weight  0.11000E+01 volume  0.68625E+02 ppm1     1.254 ppm2     3.134
ASSI (28672)
  (  segid "BrD " and resid 102  and name HD1%)
  (( segid "BrD " and resid 102  and name HA  ))
    2.100     1.100     1.100 peak 28672 weight  0.11000E+01 volume  0.69519E+03 ppm1     1.303 ppm2     4.282
ASSI (28712)
  (  segid "BrD " and resid 102  and name HD2%)
  (( segid "BrD " and resid 102  and name HB2 ))
    2.000     1.000     1.000 peak 28712 weight  0.11000E+01 volume  0.12274E+04 ppm1     1.303 ppm2     1.832
ASSI (28802)
  (( segid "BrD " and resid 115  and name HG  ))
  (( segid "BrD " and resid 115  and name HA  ))
    2.400     1.400     1.400 peak 28802 weight  0.11000E+01 volume  0.40182E+03 ppm1     2.143 ppm2     4.628
ASSI (28962)
  (  segid "BrD " and resid 56   and name HD1%)
  (( segid "BrD " and resid 34   and name HA  ))
    3.200     2.600     2.300 peak 28962 weight  0.11000E+01 volume  0.68400E+02 ppm1     1.544 ppm2     5.540
ASSI (28982)
  (( segid "BrD " and resid 59   and name HG2 ))
  (( segid "BrD " and resid 56   and name HA  ))
    2.400     1.400     1.400 peak 28982 weight  0.11000E+01 volume  0.37484E+03 ppm1     3.137 ppm2     4.636
ASSI (29062)
  (  segid "BrD " and resid 59   and name HE% )
  (( segid "BrD " and resid 56   and name HA  ))
    3.100     2.400     2.400 peak 29062 weight  0.11000E+01 volume  0.84530E+02 ppm1     1.847 ppm2     4.636
ASSI (29122)
  (  segid "BrD " and resid 59   and name HE% )
  (  segid "BrD " and resid 74   and name HE% )
    2.400     1.400     1.400 peak 29122 weight  0.11000E+01 volume  0.44730E+03 ppm1     1.848 ppm2     7.535
ASSI (29182)
  (  segid "BrD " and resid 54   and name HE% )
  (( segid "BrD " and resid 58   and name HB  ))
    3.000     2.200     2.200 peak 29182 weight  0.11000E+01 volume  0.12060E+03 ppm1     2.536 ppm2     4.696
ASSI (29282)
  (( segid "BrD " and resid 54   and name HB1 ))
  (( segid "BrD " and resid 54   and name HG1 ))
    2.800     2.000     2.000 peak 29282 weight  0.11000E+01 volume  0.16180E+03 ppm1     2.965 ppm2     3.304
ASSI (29312)
  (( segid "BrD " and resid 44   and name HB2 ))
  (( segid "BrD " and resid 44   and name HD2 ))
    3.500     3.100     2.000 peak 29312 weight  0.11000E+01 volume  0.45332E+02 ppm1     2.634 ppm2     4.126
ASSI (29342)
  (( segid "BrD " and resid 44   and name HG2 ))
  (( segid "BrD " and resid 43   and name HA  ))
    3.600     3.200     1.900 peak 29342 weight  0.11000E+01 volume  0.36619E+02 ppm1     2.645 ppm2     5.542
ASSI (29362)
  (( segid "BrD " and resid 44   and name HD1 ))
  (( segid "BrD " and resid 44   and name HA  ))
    3.200     2.600     2.300 peak 29362 weight  0.11000E+01 volume  0.69345E+02 ppm1     4.310 ppm2     5.114
ASSI (29422)
  (( segid "BrD " and resid 91   and name HB1 ))
  (( segid "BrD " and resid 91   and name HD2 ))
    2.600     1.700     1.700 peak 29422 weight  0.11000E+01 volume  0.26299E+03 ppm1     2.978 ppm2     4.407
ASSI (29432)
  (( segid "BrD " and resid 91   and name HB2 ))
  (( segid "BrD " and resid 91   and name HD2 ))
    2.800     2.000     2.000 peak 29432 weight  0.11000E+01 volume  0.15191E+03 ppm1     2.730 ppm2     4.407
ASSI (29492)
  (( segid "BrD " and resid 79   and name HG1 ))
  (( segid "BrD " and resid 76   and name HA  ))
    2.400     1.400     1.400 peak 29492 weight  0.11000E+01 volume  0.46894E+03 ppm1     3.033 ppm2     4.680
ASSI (29612)
  (( segid "BrD " and resid 70   and name HA  ))
  (  segid "BrD " and resid 69   and name HG1%)
    4.000     4.000     1.500 peak 29612 weight  0.11000E+01 volume  0.20014E+02 ppm1     5.346 ppm2     1.547
ASSI (29932)
  (( segid "BrD " and resid 66   and name HB2 ))
  (( segid "BrD " and resid 66   and name HD2 ))
    2.700     1.800     1.800 peak 29932 weight  0.11000E+01 volume  0.20564E+03 ppm1     2.641 ppm2     3.633
ASSI (29942)
  (( segid "BrD " and resid 66   and name HB1 ))
  (( segid "BrD " and resid 66   and name HD2 ))
    2.600     1.700     1.700 peak 29942 weight  0.11000E+01 volume  0.23040E+03 ppm1     2.701 ppm2     3.636
ASSI (29952)
  (( segid "BrD " and resid 66   and name HB2 ))
  (( segid "BrD " and resid 66   and name HD1 ))
    2.600     1.700     1.700 peak 29952 weight  0.11000E+01 volume  0.23393E+03 ppm1     2.633 ppm2     3.670
ASSI (29962)
  (( segid "BrD " and resid 66   and name HB1 ))
  (( segid "BrD " and resid 66   and name HD1 ))
    2.700     1.800     1.800 peak 29962 weight  0.11000E+01 volume  0.22124E+03 ppm1     2.701 ppm2     3.669
ASSI (30032)
  (( segid "BrD " and resid 51   and name HA  ))
  (( segid "BrD " and resid 52   and name HA  ))
    4.100     4.100     1.400 peak 30032 weight  0.11000E+01 volume  0.17276E+02 ppm1     4.459 ppm2     5.585
ASSI (30052)
  (( segid "BrD " and resid 86   and name HD1 ))
  (( segid "BrD " and resid 86   and name HA  ))
    3.500     3.100     2.000 peak 30052 weight  0.11000E+01 volume  0.45287E+02 ppm1     1.895 ppm2     4.810
ASSI (30162)
  (( segid "BrD " and resid 64   and name HA  ))
  (  segid "BrD " and resid 15   and name HE% )
    2.400     1.400     1.400 peak 30162 weight  0.11000E+01 volume  0.39658E+03 ppm1     4.950 ppm2     7.485
ASSI (30202)
  (( segid "BrD " and resid 64   and name HE1 ))
  (( segid "BrD " and resid 64   and name HA  ))
    2.300     1.300     1.300 peak 30202 weight  0.11000E+01 volume  0.49260E+03 ppm1     3.597 ppm2     4.939
ASSI (30342)
  (( segid "BrD " and resid 86   and name HB1 ))
  (  segid "BrD " and resid 96   and name HD% )
    2.700     1.800     1.800 peak 30342 weight  0.11000E+01 volume  0.18798E+03 ppm1     2.337 ppm2     7.722
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ASSI {30352}
  (( segid "BrD " and resid 86   and name HB1 ))
  (  segid "BrD " and resid 96   and name HB% )
     2.700     1.800     1.800 peak 30352 weight  0.11000E+01 volume  0.21345E+03 ppm1     2.338 ppm2     7.603
ASSI {30392}
  (( segid "BrD " and resid 86   and name HE1 ))
  (( segid "BrD " and resid 86   and name HA  ))
     1.100     2.400     2.400 peak 30392 weight  0.11000E+01 volume  0.90505E+02 ppm1     3.080 ppm2     4.808
ASSI {30402}
  (( segid "BrD " and resid 86   and name HE1 ))
  (( segid "BrD " and resid 86   and name HB1 ))
     2.200     1.200     1.200 peak 30402 weight  0.11000E+01 volume  0.64111E+03 ppm1     3.079 ppm2     2.370
ASSI {30412}
  (( segid "BrD " and resid 86   and name HE1 ))
  (( segid "BrD " and resid 86   and name HG1 ))
     2.300     2.100     2.100 peak 30412 weight  0.11000E+01 volume  0.14017E+03 ppm1     3.079 ppm2     1.896
ASSI {30512}
  (( segid "BrD " and resid 109  and name HE1 ))
  (( segid "BrD " and resid 109  and name HA  ))
     2.900     2.100     2.100 peak 30512 weight  0.11000E+01 volume  0.12187E+03 ppm1     3.176 ppm2     4.639
ASSI {30522}
  (( segid "BrD " and resid 109  and name HD1 ))
  (( segid "BrD " and resid 109  and name HA  ))
     1.900     0.900     0.900 peak 30522 weight  0.11000E+01 volume  0.17943E+04 ppm1     1.994 ppm2     4.639
ASSI {30622}
  (( segid "BrD " and resid 109  and name HB1 ))
  (( segid "BrD " and resid 106  and name HA  ))
     2.400     1.400     1.400 peak 30622 weight  0.11000E+01 volume  0.44758E+03 ppm1     2.334 ppm2     4.575
ASSI {30632}
  (( segid "BrD " and resid 109  and name HB2 ))
  (( segid "BrD " and resid 106  and name HA  ))
     2.700     1.800     1.800 peak 30632 weight  0.11000E+01 volume  0.21060E+03 ppm1     2.139 ppm2     4.573
ASSI {30732}
  (( segid "BrD " and resid 97   and name HG2 ))
  (( segid "BrD " and resid 97   and name HA  ))
     2.400     1.400     1.400 peak 30732 weight  0.11000E+01 volume  0.42305E+03 ppm1     2.143 ppm2     4.800
ASSI {30802}
  (( segid "BrD " and resid 104  and name HD1 ))
  (( segid "BrD " and resid 104  and name HA  ))
     1.700     0.700     0.700 peak 30802 weight  0.11000E+01 volume  0.32351E+04 ppm1     2.289 ppm2     4.671
ASSI {30862}
  (( segid "BrD " and resid 111  and name HG1 ))
  (( segid "BrD " and resid 111  and name HA  ))
     2.500     1.600     1.600 peak 30862 weight  0.11000E+01 volume  0.32568E+03 ppm1     2.000 ppm2     4.670
ASSI {30872}
  (( segid "BrD " and resid 111  and name HD1 ))
  (( segid "BrD " and resid 111  and name HA  ))
     2.500     1.600     1.600 peak 30872 weight  0.11000E+01 volume  0.34175E+03 ppm1     2.240 ppm2     4.656
ASSI {30912}
  (( segid "BrD " and resid 111  and name HE1 ))
  (( segid "BrD " and resid 111  and name HA  ))
     2.200     1.200     1.200 peak 30912 weight  0.11000E+01 volume  0.72636E+03 ppm1     3.520 ppm2     4.656
ASSI {31022}
  (( segid "BrD " and resid 72   and name HD1 ))
  (( segid "BrD " and resid 72   and name HE2 ))
     2.200     1.200     1.200 peak 31022 weight  0.11000E+01 volume  0.72521E+03 ppm1     2.287 ppm2     3.654
ASSI {31032}
  (( segid "BrD " and resid 72   and name HD1 ))
  (( segid "BrD " and resid 72   and name HE1 ))
     2.300     1.300     1.300 peak 31032 weight  0.11000E+01 volume  0.50216E+03 ppm1     2.287 ppm2     3.744
ASSI {31042}
  (( segid "BrD " and resid 72   and name HB1 ))
  (( segid "BrD " and resid 72   and name HE1 ))
     2.200     1.200     1.200 peak 31042 weight  0.11000E+01 volume  0.79378E+03 ppm1     2.387 ppm2     3.744
ASSI {31052}
  (( segid "BrD " and resid 72   and name HB1 ))
  (( segid "BrD " and resid 72   and name HE2 ))
     1.900     0.900     0.900 peak 31052 weight  0.11000E+01 volume  0.15518E+04 ppm1     2.386 ppm2     3.652
ASSI { 1632}
  (  segid "BrD " and resid 110  and name HD1% )
  (( segid "BrD " and resid 78   and name HB1 ))
     2.100     2.100     2.400 peak  1632 weight  0.10000E+01 volume  0.10163E+04 ppm1     1.154 ppm2     1.309
ASSI { 4042}
  (( segid "BrD " and resid 79   and name HG1 ))
  (( segid "BrD " and resid 80   and name HG1 ))
     3.700     3.400     1.800 peak  4042 weight  0.10000E+01 volume  0.30439E+02 ppm1     3.029 ppm2     2.351
ASSI { 4882}
  (( segid "BrD " and resid 19   and name HD1 ))
  (  segid "BrD " and resid 63   and name HD2% )
     2.700     1.800     1.800 peak  4882 weight  0.10000E+01 volume  0.22363E+03 ppm1     2.191 ppm2     1.495
ASSI { 4902}
  (( segid "BrD " and resid 97   and name HB1 ))
  (  segid "BrD " and resid 101  and name HD1% )
     3.000     2.200     2.200 peak  4902 weight  0.10000E+01 volume  0.10809E+03 ppm1     2.683 ppm2     1.580
ASSI { 4992}
  (( segid "BrD " and resid 37   and name HG2 ))
  (( segid "BrD " and resid 55   and name HA  ))
     4.200     4.200     1.300 peak  4992 weight  0.10000E+01 volume  0.14817E+02 ppm1     2.586 ppm2     5.380
ASSI { 6092}
  (( segid "BrD " and resid 115  and name HG  ))
  (  segid "BrD " and resid 110  and name HG2% )
     3.700     3.400     1.800 peak  6092 weight  0.10000E+01 volume  0.29496E+02 ppm1     2.140 ppm2     1.222
ASSI { 6222}
  (  segid "BrD " and resid 22   and name HD2% )
  (  segid "BrD " and resid 56   and name HD2% )
     2.300     1.300     1.300 peak  6222 weight  0.10000E+01 volume  0.52799E+03 ppm1     1.599 ppm2     1.246
ASSI { 6602}
  (  segid "BrD " and resid 31   and name HB% )
  (  segid "BrD " and resid 56   and name HD1% )
     2.500     1.600     1.600 peak  6602 weight  0.10000E+01 volume  0.36161E+03 ppm1     2.291 ppm2     1.539
ASSI { 6792}
  (  segid "BrD " and resid 99   and name HB% )
  (( segid "BrD " and resid 82   and name HA  ))
     3.000     2.200     2.200 peak  6792 weight  0.10000E+01 volume  0.12038E+03 ppm1     2.190 ppm2     4.752
ASSI { 6832}
  (  segid "BrD " and resid 99   and name HB% )
  (( segid "BrD " and resid 86   and name HG2 ))
     3.000     2.200     2.200 peak  6832 weight  0.10000E+01 volume  0.11935E+03 ppm1     2.191 ppm2     0.765
ASSI { 6852}
  (  segid "BrD " and resid 113  and name HB% )
  (  segid "BrD " and resid 110  and name HG2% )
     2.800     2.000     2.000 peak  6852 weight  0.10000E+01 volume  0.15622E+03 ppm1     1.991 ppm2     1.221
ASSI { 6862}
  (  segid "BrD " and resid 113  and name HB% )
  (  segid "BrD " and resid 18   and name HD1% )
     4.900     4.900     0.600 peak  6862 weight  0.10000E+01 volume  0.56980E+01 ppm1     1.991 ppm2     1.066
ASSI { 6902}
  (( segid "BrD " and resid 31   and name HA  ))
  (( segid "BrD " and resid 33   and name HD1 ))
     3.200     2.700     2.200 peak  6902 weight  0.10000E+01 volume  0.60152E+02 ppm1     5.000 ppm2     2.794
ASSI { 6952}
  (  segid "BrD " and resid 25   and name HG2% )
  (  segid "BrD " and resid 31   and name HB% )
     2.500     1.600     1.600 peak  6952 weight  0.10000E+01 volume  0.32952E+03 ppm1     1.650 ppm2     2.320
ASSI { 6982}
  (  segid "BrD " and resid 25   and name HG2% )
  (  segid "BrD " and resid 56   and name HD2% )
     2.500     1.600     1.600 peak  6982 weight  0.10000E+01 volume  0.36117E+03 ppm1     1.646 ppm2     1.252
ASSI { 7362}
  (  segid "BrD " and resid 25   and name HG2% )
  (( segid "BrD " and resid 102  and name HG  ))
     2.900     2.100     2.100 peak  7362 weight  0.10000E+01 volume  0.13044E+03 ppm1     1.647 ppm2     2.157
ASSI { 7412}
  (( segid "BrD " and resid 46   and name HA  ))
  (  segid "BrD " and resid 49   and name HG1% )
     3.400     2.900     2.100 peak  7412 weight  0.10000E+01 volume  0.55913E+02 ppm1     4.164 ppm2     1.645
ASSI { 7422}
  (( segid "BrD " and resid 46   and name HA  ))
  (  segid "BrD " and resid 43   and name HB% )
     3.600     3.200     1.900 peak  7422 weight  0.10000E+01 volume  0.39252E+02 ppm1     4.164 ppm2     1.718
ASSI { 7442}
  (( segid "BrD " and resid 68   and name HA  ))
  (  segid "BrD " and resid 63   and name HD1% )
     3.700     3.400     1.800 peak  7442 weight  0.10000E+01 volume  0.32100E+02 ppm1     5.146 ppm2     1.653
ASSI { 7462}
  (( segid "BrD " and resid 68   and name HB2 ))
  (  segid "BrD " and resid 18   and name HD1% )
     3.100     2.400     2.400 peak  7462 weight  0.10000E+01 volume  0.95501E+02 ppm1     3.522 ppm2     1.083
ASSI { 7472}
  (( segid "BrD " and resid 68   and name HB1 ))
  (  segid "BrD " and resid 18   and name HD1% )
     3.100     2.600     2.400 peak  7472 weight  0.10000E+01 volume  0.86786E+02 ppm1     3.669 ppm2     1.084
ASSI { 8082}
  (( segid "BrD " and resid 98   and name HA  ))
  (( segid "BrD " and resid 30   and name HB2 ))
     2.900     2.100     2.100 peak  8082 weight  0.10000E+01 volume  0.14301E+03 ppm1     4.802 ppm2     4.530
ASSI { 8132}
  (  segid "BrD " and resid 63   and name HD1% )
  (( segid "BrD " and resid 15   and name HA  ))
     2.800     2.000     2.000 peak  8132 weight  0.10000E+01 volume  0.17717E+03 ppm1     1.646 ppm2     6.624
ASSI { 8252}
  (( segid "BrD " and resid 109  and name HG1 ))
  (( segid "BrD " and resid 109  and name HD1 ))
     2.700     1.800     1.800 peak  8252 weight  0.10000E+01 volume  0.20695E+03 ppm1     1.401 ppm2     1.989
ASSI { 8282}
  (( segid "BrD " and resid 18   and name HA  ))
  (( segid "BrD " and resid 21   and name HG12 ))
     3.300     2.700     2.200 peak  8282 weight  0.10000E+01 volume  0.61204E+02 ppm1     3.866 ppm2     1.640
ASSI { 8362}
  (( segid "BrD " and resid 18   and name HG  ))
  (  segid "BrD " and resid 14   and name HD2% )
     3.100     2.400     2.400 peak  8362 weight  0.10000E+01 volume  0.89516E+02 ppm1     2.290 ppm2     1.418
OR { 8362}
  (( segid "BrD " and resid 18   and name HG  ))
  (  segid "BrD " and resid 14   and name HD1% )
ASSI { 8422}
  (  segid "BrD " and resid 18   and name HD1% )
  (( segid "BrD " and resid 14   and name HG  ))
     2.700     1.800     1.800 peak  8422 weight  0.10000E+01 volume  0.21908E+03 ppm1     1.068 ppm2     3.070
ASSI { 8432}
  (  segid "BrD " and resid 18   and name HD1% )
  (( segid "BrD " and resid 15   and name HA  ))
     2.700     1.800     1.800 peak  8432 weight  0.10000E+01 volume  0.20923E+03 ppm1     1.057 ppm2     4.626
ASSI { 8512}
  (  segid "BrD " and resid 22   and name HD2% )
  (  segid "BrD " and resid 78   and name HD2% )
     3.300     2.700     2.200 peak  8512 weight  0.10000E+01 volume  0.62220E+02 ppm1     1.599 ppm2     0.677
ASSI { 8522}
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   (  segid "BrD " and resid 22   and name HD2%)
   (  segid "BrD " and resid 59   and name HE% )
      2.900     2.100     2.100 peak  8522 weight  0.10000E+01 volume  0.12491E+03 ppm1      1.599 ppm2      1.671
ASSI [ 8532]
   (  segid "BrD " and resid 22   and name HD1%)
   (( segid "BrD " and resid 60   and name HA  ))
      2.600     1.700     1.700 peak  8532 weight  0.10000E+01 volume  0.23265E+03 ppm1      1.645 ppm2      4.809
ASSI [ 8582]
   (( segid "BrD " and resid 22   and name HB2 ))
   (  segid "BrD " and resid 63   and name HD2%)
      2.600     1.700     1.700 peak  8582 weight  0.10000E+01 volume  0.24738E+03 ppm1      2.286 ppm2      1.494
ASSI [ 8612]
   (( segid "BrD " and resid 56   and name HB1 ))
   (( segid "BrD " and resid 35   and name HA  ))
      2.800     2.000     2.000 peak  8612 weight  0.10000E+01 volume  0.17130E+03 ppm1      2.685 ppm2      4.900
ASSI [ 8632]
   (  segid "BrD " and resid 56   and name HD1%)
   (  segid "BrD " and resid 81   and name HG2%)
      3.800     3.600     1.700 peak  8632 weight  0.10000E+01 volume  0.24706E+02 ppm1      1.547 ppm2      0.758
ASSI [ 8642]
   (( segid "BrD " and resid 116  and name HG12))
   (( segid "BrD " and resid 116  and name HG11))
      2.000     1.000     1.000 peak  8642 weight  0.10000E+01 volume  0.13013E+04 ppm1      1.548 ppm2      1.921
ASSI [ 8702]
   (  segid "BrD " and resid 56   and name HD2%)
   (  segid "BrD " and resid 81   and name HG1%)
      2.400     1.400     1.400 peak  8702 weight  0.10000E+01 volume  0.46717E+03 ppm1      1.254 ppm2      1.080
ASSI [ 8832]
   (  segid "BrD " and resid 78   and name HD1%)
   (( segid "BrD " and resid 18   and name HB2 ))
      4.100     4.100     1.400 peak  8832 weight  0.10000E+01 volume  0.15698E+02 ppm1      0.761 ppm2      0.924
ASSI [ 8862]
   (  segid "BrD " and resid 78   and name HD2%)
   (  segid "BrD " and resid 18   and name HD2%)
      3.000     2.200     2.200 peak  8862 weight  0.10000E+01 volume  0.10893E+03 ppm1      0.662 ppm2      0.427
ASSI [ 8942]
   (( segid "BrD " and resid 102  and name HA  ))
   (  segid "BrD " and resid 101  and name HG2%)
      3.100     2.400     2.400 peak  8942 weight  0.10000E+01 volume  0.83720E+02 ppm1      4.263 ppm2      1.612
ASSI [ 9102]
   (( segid "BrD " and resid 21   and name HG12))
   (  segid "BrD " and resid 102  and name HD2%)
      3.700     3.400     1.800 peak  9102 weight  0.10000E+01 volume  0.31128E+02 ppm1      1.648 ppm2      1.320
OR [ 9102]
   (( segid "BrD " and resid 21   and name HG12))
   (  segid "BrD " and resid 102  and name HD1%)
ASSI [ 9122]
   (  segid "BrD " and resid 21   and name HG2%)
   (  segid "BrD " and resid 110  and name HD1%)
      2.900     2.100     2.100 peak  9122 weight  0.10000E+01 volume  0.12723E+03 ppm1      1.600 ppm2      1.143
ASSI [ 9132]
   (  segid "BrD " and resid 21   and name HG2%)
   (  segid "BrD " and resid 78   and name HD2%)
      3.400     2.900     2.100 peak  9132 weight  0.10000E+01 volume  0.50284E+02 ppm1      1.596 ppm2      0.670
ASSI [ 9172]
   (  segid "BrD " and resid 21   and name HD1%)
   (  segid "BrD " and resid 17   and name HG2%)
      2.500     1.600     1.600 peak  9172 weight  0.10000E+01 volume  0.33280E+03 ppm1      1.205 ppm2      1.748
ASSI [ 9402]
   (  segid "BrD " and resid 21   and name HG2%)
   (( segid "BrD " and resid 106  and name HA  ))
      2.600     1.700     1.700 peak  9402 weight  0.10000E+01 volume  0.25016E+03 ppm1      1.597 ppm2      4.536
ASSI [ 9412]
   (  segid "BrD " and resid 101  and name HG2%)
   (( segid "BrD " and resid 30   and name HB1 ))
      2.800     2.000     2.000 peak  9412 weight  0.10000E+01 volume  0.17182E+03 ppm1      1.598 ppm2      4.928
ASSI [ 9462]
   (( segid "BrD " and resid 110  and name HB  ))
   (( segid "BrD " and resid 115  and name HB1 ))
      3.000     2.200     2.200 peak  9462 weight  0.10000E+01 volume  0.11040E+03 ppm1      2.338 ppm2      2.182
ASSI [ 9502]
   (  segid "BrD " and resid 110  and name HG2%)
   (( segid "BrD " and resid 115  and name HB1 ))
      2.500     1.600     1.600 peak  9502 weight  0.10000E+01 volume  0.34762E+03 ppm1      1.252 ppm2      2.182
ASSI [ 9512]
   (  segid "BrD " and resid 110  and name HG2%)
   (( segid "BrD " and resid 116  and name HG12))
      2.500     1.600     1.600 peak  9512 weight  0.10000E+01 volume  0.33973E+03 ppm1      1.253 ppm2      1.586
ASSI [ 9572]
   (  segid "BrD " and resid 110  and name HD1%)
   (  segid "BrD " and resid 78   and name HD1%)
      3.800     3.600     1.700 peak  9572 weight  0.10000E+01 volume  0.27664E+02 ppm1      1.154 ppm2      0.750
ASSI [ 9602]
   (  segid "BrD " and resid 110  and name HD1%)
   (  segid "BrD " and resid 78   and name HD2%)
      3.400     2.900     2.100 peak  9602 weight  0.10000E+01 volume  0.49420E+02 ppm1      1.154 ppm2      0.676
ASSI [ 9622]
   (  segid "BrD " and resid 116  and name HG2%)
   (  segid "BrD " and resid 110  and name HG2%)
      2.800     2.000     2.000 peak  9622 weight  0.10000E+01 volume  0.18357E+03 ppm1      1.401 ppm2      1.271
ASSI [ 9632]
   (  segid "BrD " and resid 116  and name HD1%)
   (  segid "BrD " and resid 110  and name HD1%)
      2.100     1.100     1.100 peak  9632 weight  0.10000E+01 volume  0.89032E+03 ppm1      1.399 ppm2      1.152
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ASSI [ 9992]
   (( segid "BrD " and resid 56   and name HB2 ))
   (( segid "BrD " and resid 59   and name HB2 ))
      2.700     1.800     1.800 peak  9992 weight  0.10000E+01 volume  0.19570E+03 ppm1      1.947 ppm2      2.490
ASSI [10032]
   (( segid "BrD " and resid 56   and name HA  ))
   (( segid "BrD " and resid 59   and name HB2 ))
      3.000     2.200     2.200 peak 10032 weight  0.10000E+01 volume  0.99741E+02 ppm1      5.541 ppm2      2.481
ASSI [10142]
   (( segid "BrD " and resid 70   and name HB2 ))
   (( segid "BrD " and resid 73   and name HB1 ))
      4.100     4.100     1.400 peak 10142 weight  0.10000E+01 volume  0.17585E+02 ppm1      4.360 ppm2      2.597
ASSI [10172]
   (( segid "BrD " and resid 52   and name HB2 ))
   (( segid "BrD " and resid 80   and name HG1 ))
      4.200     4.200     1.300 peak 10172 weight  0.10000E+01 volume  0.15368E+02 ppm1      3.522 ppm2      2.345
ASSI [10512]
   (( segid "BrD " and resid 61   and name HG1 ))
   (( segid "BrD " and resid 60   and name HB2 ))
      2.700     1.800     1.800 peak 10512 weight  0.10000E+01 volume  0.19616E+03 ppm1      2.980 ppm2      4.586
ASSI [10832]
   (( segid "BrD " and resid 30   and name HB1 ))
   (  segid "BrD " and resid 102  and name HD1%)
      3.600     3.200     1.900 peak 10832 weight  0.10000E+01 volume  0.34957E+02 ppm1      4.907 ppm2      1.329
ASSI [10842]
   (( segid "BrD " and resid 30   and name HB2 ))
   (  segid "BrD " and resid 102  and name HD1%)
      3.200     2.600     2.300 peak 10842 weight  0.10000E+01 volume  0.80809E+02 ppm1      4.510 ppm2      1.320
ASSI [10912]
   (( segid "BrD " and resid 93   and name HB1 ))
   (( segid "BrD " and resid 91   and name HG1 ))
      3.700     3.400     1.800 peak 10912 weight  0.10000E+01 volume  0.32596E+02 ppm1      5.000 ppm2      2.798
ASSI [10922]
   (( segid "BrD " and resid 93   and name HB2 ))
   (( segid "BrD " and resid 91   and name HG1 ))
      3.700     3.400     1.800 peak 10922 weight  0.10000E+01 volume  0.31695E+02 ppm1      4.755 ppm2      2.799
ASSI [10962]
   (( segid "BrD " and resid 44   and name HA  ))
   (( segid "BrD " and resid 41   and name HA  ))
      4.600     4.600     0.900 peak 10962 weight  0.10000E+01 volume  0.78869E+01 ppm1      5.099 ppm2      4.654
ASSI [11342]
   (( segid "BrD " and resid 19   and name HG1 ))
   (  segid "BrD " and resid 63   and name HD2%)
      3.100     2.400     2.400 peak 11342 weight  0.10000E+01 volume  0.91996E+02 ppm1      1.889 ppm2      1.493
ASSI [11372]
   (( segid "BrD " and resid 26   and name HA  ))
   (  segid "BrD " and resid 31   and name HB% )
      2.200     1.200     1.200 peak 11372 weight  0.10000E+01 volume  0.67300E+03 ppm1      4.509 ppm2      2.311
ASSI [11382]
   (( segid "BrD " and resid 26   and name HA  ))
   (  segid "BrD " and resid 35   and name HE% )
      2.800     2.000     2.000 peak 11382 weight  0.10000E+01 volume  0.18352E+03 ppm1      4.509 ppm2      2.783
ASSI [11502]
   (( segid "BrD " and resid 86   and name HE1 ))
   (( segid "BrD " and resid 83   and name HA  ))
      2.900     2.100     2.100 peak 11502 weight  0.10000E+01 volume  0.14787E+03 ppm1      3.080 ppm2      4.460
ASSI [11572]
   (( segid "BrD " and resid 109  and name HB1 ))
   (  segid "BrD " and resid 21   and name HG2%)
      3.500     3.100     2.000 peak 11572 weight  0.10000E+01 volume  0.46116E+02 ppm1      2.334 ppm2      1.587
ASSI [11642]
   (( segid "BrD " and resid 6    and name HB2 ))
   (( segid "BrD " and resid 7    and name HG1 ))
      3.100     2.400     2.400 peak 11642 weight  0.10000E+01 volume  0.90515E+02 ppm1      2.291 ppm2      2.876
ASSI [11752]
   (( segid "BrD " and resid 55   and name HB1 ))
   (( segid "BrD " and resid 37   and name HA  ))
      2.600     2.000     2.000 peak 11752 weight  0.10000E+01 volume  0.16032E+03 ppm1      2.979 ppm2      4.860
ASSI [11832]
   (( segid "BrD " and resid 91   and name HA  ))
   (( segid "BrD " and resid 92   and name HB2 ))
      3.500     3.100     2.000 peak 11832 weight  0.10000E+01 volume  0.43713E+02 ppm1      5.347 ppm2      2.571
ASSI [12292]
   (  segid "BrD " and resid 81   and name HG2%)
   (( segid "BrD " and resid 56   and name HG  ))
      3.300     2.700     2.200 peak 12292 weight  0.10000E+01 volume  0.58134E+02 ppm1      0.761 ppm2      2.323
ASSI [12502]
   (( segid "BrD " and resid 54   and name HG1 ))
   (( segid "BrD " and resid 59   and name HB2 ))
      4.000     4.000     1.500 peak 12502 weight  0.10000E+01 volume  0.18992E+02 ppm1      3.288 ppm2      2.467
ASSI [12632]
   (  segid "BrD " and resid 59   and name HE% )
   (( segid "BrD " and resid 77   and name HB1 ))
      2.500     1.600     1.600 peak 12632 weight  0.10000E+01 volume  0.30644E+03 ppm1      1.848 ppm2      3.321
ASSI [12732]
   (( segid "BrD " and resid 71   and name HA  ))
   (  segid "BrD " and resid 18   and name HD1%)
      3.700     3.400     1.800 peak 12732 weight  0.10000E+01 volume  0.29522E+02 ppm1      4.608 ppm2      1.084
ASSI [12752]
   (( segid "BrD " and resid 71   and name HA  ))
   (  segid "BrD " and resid 18   and name HD2%)
      3.300     2.700     2.200 peak 12752 weight  0.10000E+01 volume  0.66213E+02 ppm1      4.607 ppm2      0.409
ASSI [12872]
   (( segid "BrD " and resid 62   and name HD1 ))
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   (( segid "BrD " and resid 59   and name HB2 ))
      3.500     3.100     2.000 peak 12872 weight  0.10000E+01 volume  0.44954E+02 ppm1      3.177 ppm2      2.484
ASSI {13092}
   (( segid "BrD " and resid 54   and name HG1 ))
   ( segid "BrD " and resid 81   and name HG1%)
      3.400     2.900     2.100 peak 13092 weight  0.10000E+01 volume  0.51686E+02 ppm1      3.288 ppm2      1.075
ASSI {13112}
   (( segid "BrD " and resid 73   and name HB2 ))
   (( segid "BrD " and resid 68   and name HA  ))
      3.000     2.200     2.200 peak 13112 weight  0.10000E+01 volume  0.10760E+03 ppm1      2.486 ppm2      5.142
ASSI {13122}
   (( segid "BrD " and resid 73   and name HB1 ))
   (( segid "BrD " and resid 68   and name HA  ))
      2.900     2.100     2.100 peak 13122 weight  0.10000E+01 volume  0.13268E+03 ppm1      2.583 ppm2      5.141
ASSI {13232}
   (( segid "BrD " and resid 46   and name HB1 ))
   ( segid "BrD " and resid 38   and name HG2%)
      3.500     3.100     2.000 peak 13232 weight  0.10000E+01 volume  0.45934E+02 ppm1      3.275 ppm2      0.790
ASSI {13282}
   (( segid "BrD " and resid 56   and name HA  ))
   ( segid "BrD " and resid 22   and name HD2%)
      3.100     2.400     2.400 peak 13282 weight  0.10000E+01 volume  0.86018E+02 ppm1      4.607 ppm2      1.637
OR {13282}
   (( segid "BrD " and resid 56   and name HA  ))
   ( segid "BrD " and resid 22   and name HD1%)
ASSI {13312}
   (( segid "BrD " and resid 116  and name HG12))
   ( segid "BrD " and resid 110  and name HD1%)
      2.700     1.800     1.800 peak 13312 weight  0.10000E+01 volume  0.18778E+03 ppm1      1.548 ppm2      1.145
ASSI {13332}
   ( segid "BrD " and resid 22   and name HD1%)
   (( segid "BrD " and resid 63   and name HB2 ))
      2.500     1.600     1.600 peak 13332 weight  0.10000E+01 volume  0.34390E+03 ppm1      1.648 ppm2      2.516
ASSI {13412}
   ( segid "BrD " and resid 25   and name HG1%)
   ( segid "BrD " and resid 56   and name HD2%)
      2.900     2.100     2.100 peak 13412 weight  0.10000E+01 volume  0.12726E+03 ppm1      1.795 ppm2      1.252
ASSI {13572}
   (( segid "BrD " and resid 49   and name HB  ))
   (( segid "BrD " and resid 50   and name HG11))
      5.500     5.500     0.000 peak 13572 weight  0.10000E+01 volume  0.27123E-01 ppm1      2.634 ppm2      1.417
ASSI {13582}
   (( segid "BrD " and resid 49   and name HB  ))
   ( segid "BrD " and resid 50   and name HD1%)
      4.000     4.000     1.500 peak 13582 weight  0.10000E+01 volume  0.18896E+02 ppm1      2.634 ppm2      1.148
ASSI {13682}
   ( segid "BrD " and resid 54   and name HE% )
   (( segid "BrD " and resid 57   and name HG1 ))
      3.600     3.200     1.900 peak 13682 weight  0.10000E+01 volume  0.37432E+02 ppm1      2.537 ppm2      2.101
ASSI {13732}
   (( segid "BrD " and resid 63   and name HA  ))
   (( segid "BrD " and resid 68   and name HB1 ))
      3.500     3.100     2.000 peak 13732 weight  0.10000E+01 volume  0.44471E+02 ppm1      5.296 ppm2      3.662
ASSI {13752}
   ( segid "BrD " and resid 63   and name HD2%)
   (( segid "BrD " and resid 19   and name HB2 ))
      2.700     1.800     1.800 peak 13752 weight  0.10000E+01 volume  0.20264E+03 ppm1      1.498 ppm2      1.996
ASSI {13772}
   (( segid "BrD " and resid 64   and name HA  ))
   ( segid "BrD " and resid 63   and name HD2%)
      4.000     4.000     1.500 peak 13772 weight  0.10000E+01 volume  0.18294E+02 ppm1      4.951 ppm2      1.488
ASSI {13792}
   ( segid "BrD " and resid 49   and name HG1%)
   ( segid "BrD " and resid 50   and name HG2%)
      3.800     3.600     1.700 peak 13792 weight  0.10000E+01 volume  0.26015E+02 ppm1      1.646 ppm2      1.009
ASSI {13812}
   (( segid "BrD " and resid 76   and name HA  ))
   (( segid "BrD " and resid 80   and name HB2 ))
      4.200     4.200     1.300 peak 13812 weight  0.10000E+01 volume  0.14556E+02 ppm1      4.656 ppm2      2.508
ASSI {13832}
   (( segid "BrD " and resid 56   and name HB1 ))
   (( segid "BrD " and resid 34   and name HB2 ))
      3.100     2.400     2.400 peak 13832 weight  0.10000E+01 volume  0.92421E+02 ppm1      2.685 ppm2      3.159
ASSI {13842}
   (( segid "BrD " and resid 67   and name HB2 ))
   (( segid "BrD " and resid 62   and name HA  ))
      3.400     2.900     2.100 peak 13842 weight  0.10000E+01 volume  0.56015E+02 ppm1      2.636 ppm2      4.483
ASSI {13862}
   ( segid "BrD " and resid 69   and name HG2%)
   ( segid "BrD " and resid 18   and name HD1%)
      3.600     3.200     1.900 peak 13862 weight  0.10000E+01 volume  0.35688E+02 ppm1      1.425 ppm2      1.030
ASSI {13872}
   ( segid "BrD " and resid 69   and name HG2%)
   (( segid "BrD " and resid 18   and name HB2 ))
      5.500     5.500     0.000 peak 13872 weight  0.10000E+01 volume  0.14355E+01 ppm1      1.425 ppm2      0.880
ASSI {13892}
   (( segid "BrD " and resid 12   and name HA  ))
   ( segid "BrD " and resid 14   and name HD2%)
      3.000     2.200     2.200 peak 13892 weight  0.10000E+01 volume  0.11539E+03 ppm1      5.298 ppm2      1.382
OR {13892}
   (( segid "BrD " and resid 12   and name HA  ))
   ( segid "BrD " and resid 14   and name HD1%)
ASSI {13982}
   (( segid "BrD " and resid 74   and name HA  ))
   (( segid "BrD " and resid 68   and name HB2 ))
      3.600     3.200     1.900 peak 13982 weight  0.10000E+01 volume  0.36366E+02 ppm1      4.360 ppm2      3.499
ASSI {14032}
   ( segid "BrD " and resid 76   and name HB% )
   (( segid "BrD " and resid 80   and name HG1 ))
      2.800     2.000     2.000 peak 14032 weight  0.10000E+01 volume  0.17964E+03 ppm1      2.091 ppm2      2.344
ASSI {14052}
   ( segid "BrD " and resid 14   and name HD1%)
   (( segid "BrD " and resid 70   and name HA  ))
      2.700     1.800     1.800 peak 14052 weight  0.10000E+01 volume  0.21486E+03 ppm1      1.402 ppm2      5.362
ASSI {14112}
   (( segid "BrD " and resid 14   and name HA  ))
   ( segid "BrD " and resid 113  and name HB% )
      3.100     2.400     2.400 peak 14112 weight  0.10000E+01 volume  0.82177E+02 ppm1      4.655 ppm2      1.987
ASSI {14212}
   (( segid "BrD " and resid 98   and name HB2 ))
   (( segid "BrD " and resid 30   and name HB1 ))
      3.700     3.400     1.800 peak 14212 weight  0.10000E+01 volume  0.32251E+02 ppm1      3.667 ppm2      4.933
ASSI {14222}
   (( segid "BrD " and resid 99   and name HA  ))
   (( segid "BrD " and resid 102  and name HG  ))
      3.400     2.900     2.100 peak 14222 weight  0.10000E+01 volume  0.54061E+02 ppm1      4.459 ppm2      2.136
ASSI {14242}
   (( segid "BrD " and resid 98   and name HA  ))
   (( segid "BrD " and resid 62   and name HB2 ))
      3.000     2.200     2.200 peak 14242 weight  0.10000E+01 volume  0.10335E+03 ppm1      4.457 ppm2      3.561
ASSI {14262}
   (( segid "BrD " and resid 31   and name HA  ))
   (( segid "BrD " and resid 31   and name HD2 ))
      3.300     2.700     2.200 peak 14262 weight  0.10000E+01 volume  0.61370E+02 ppm1      5.000 ppm2      2.218
ASSI {14272}
   ( segid "BrD " and resid 31   and name HB% )
   (( segid "BrD " and resid 25   and name HA  ))
      3.000     2.200     2.200 peak 14272 weight  0.10000E+01 volume  0.10586E+03 ppm1      2.289 ppm2      4.437
ASSI {14292}
   (( segid "BrD " and resid 110  and name HB  ))
   ( segid "BrD " and resid 115  and name HD1%)
      5.500     5.500     0.000 peak 14292 weight  0.10000E+01 volume  0.49515E+00 ppm1      2.338 ppm2      1.318
ASSI {14302}
   ( segid "BrD " and resid 63   and name HD2%)
   (( segid "BrD " and resid 22   and name HB1 ))
      2.500     1.600     1.600 peak 14302 weight  0.10000E+01 volume  0.30120E+03 ppm1      1.498 ppm2      2.695
ASSI {14332}
   (( segid "BrD " and resid 103  and name HA  ))
   (( segid "BrD " and resid 102  and name HB2 ))
      3.500     3.100     2.000 peak 14332 weight  0.10000E+01 volume  0.41084E+02 ppm1      3.769 ppm2      1.830
ASSI {14352}
   (( segid "BrD " and resid 106  and name HA  ))
   (( segid "BrD " and resid 109  and name HG1 ))
      4.000     4.000     1.500 peak 14352 weight  0.10000E+01 volume  0.19913E+02 ppm1      4.555 ppm2      1.435
ASSI {14382}
   (( segid "BrD " and resid 15   and name HA  ))
   (( segid "BrD " and resid 14   and name HG  ))
      3.800     3.600     1.700 peak 14382 weight  0.10000E+01 volume  0.25435E+02 ppm1      4.606 ppm2      2.042
ASSI {14442}
   (( segid "BrD " and resid 110  and name HA  ))
   (( segid "BrD " and resid 115  and name HB1 ))
      2.800     2.000     2.000 peak 14442 weight  0.10000E+01 volume  0.18018E+03 ppm1      4.411 ppm2      2.181
OR {14442}
   (( segid "BrD " and resid 110  and name HA  ))
   (( segid "BrD " and resid 115  and name HG  ))
ASSI {14452}
   ( segid "BrD " and resid 110  and name HG2%)
   ( segid "BrD " and resid 115  and name HD1%)
      2.600     1.700     1.700 peak 14452 weight  0.10000E+01 volume  0.23487E+03 ppm1      1.254 ppm2      1.330
ASSI {14512}
   (( segid "BrD " and resid 111  and name HG1 ))
   ( segid "BrD " and resid 110  and name HG2%)
      3.600     3.200     1.900 peak 14512 weight  0.10000E+01 volume  0.36391E+02 ppm1      1.989 ppm2      1.278
ASSI {14652}
   (( segid "BrD " and resid 18   and name HA  ))
   (( segid "BrD " and resid 21   and name HG11))
      3.700     3.400     1.800 peak 14652 weight  0.10000E+01 volume  0.30202E+02 ppm1      3.866 ppm2      2.351
ASSI {14672}
   ( segid "BrD " and resid 18   and name HD1%)
   (( segid "BrD " and resid 63   and name HG  ))
      3.100     2.400     2.400 peak 14672 weight  0.10000E+01 volume  0.91159E+02 ppm1      1.057 ppm2      2.467
ASSI {14702}
   ( segid "BrD " and resid 21   and name HD1%)
   ( segid "BrD " and resid 63   and name HD2%)
      2.300     2.300     2.200 peak 14702 weight  0.10000E+01 volume  0.60922E+03 ppm1      1.205 ppm2      1.458
ASSI {14752}
   ( segid "BrD " and resid 54   and name HE% )
   ( segid "BrD " and resid 81   and name HG1%)
      3.700     3.400     1.800 peak 14752 weight  0.10000E+01 volume  0.28669E+02 ppm1      2.535 ppm2      1.075
ASSI {14762}
   (( segid "BrD " and resid 51   and name HA  ))
   (( segid "BrD " and resid 53   and name HD1 ))
      5.500     5.500     0.000 peak 14762 weight  0.10000E+01 volume  0.89215E-01 ppm1      4.460 ppm2      4.222
ASSI {14782}
   (( segid "BrD " and resid 36   and name HA  ))
   (( segid "BrD " and resid 57   and name HB1 ))
      2.300     1.300     1.300 peak 14782 weight  0.10000E+01 volume  0.60436E+03 ppm1      5.446 ppm2      3.986
ASSI {15012}
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   (( segid "BrD " and resid 46   and name HB1 ))
   (  segid "BrD " and resid 38   and name HG1%)
      4.000     4.000     1.500 peak 15012 weight  0.10000E+01 volume  0.20055E+02 ppm1      3.275 ppm2      1.075
ASSI {15032}
   (( segid "BrD " and resid 46   and name HB1 ))
   (  segid "BrD " and resid 47   and name HD% )
      4.500     4.500     1.000 peak 15032 weight  0.10000E+01 volume  0.96365E+01 ppm1      3.276 ppm2      7.934
ASSI {15042}
   (( segid "BrD " and resid 46   and name HB2 ))
   (  segid "BrD " and resid 47   and name HD% )
      3.200     2.600     2.300 peak 15042 weight  0.10000E+01 volume  0.71990E+02 ppm1      3.077 ppm2      7.933
ASSI {15052}
   (( segid "BrD " and resid 46   and name HA  ))
   (  segid "BrD " and resid 49   and name HG2%)
      3.600     3.200     1.900 peak 15052 weight  0.10000E+01 volume  0.38868E+02 ppm1      4.165 ppm2      1.571
ASSI {15092}
   (( segid "BrD " and resid 28   and name HB2 ))
   (  segid "BrD " and resid 31   and name HB% )
      2.800     2.000     2.000 peak 15092 weight  0.10000E+01 volume  0.15966E+03 ppm1      3.374 ppm2      2.312
ASSI {15182}
   (( segid "BrD " and resid 67   and name HB1 ))
   (( segid "BrD " and resid 62   and name HB2 ))
      4.000     4.000     1.500 peak 15182 weight  0.10000E+01 volume  0.19603E+02 ppm1      3.572 ppm2      1.693
ASSI {15192}
   (( segid "BrD " and resid 67   and name HB1 ))
   (( segid "BrD " and resid 62   and name HG2 ))
      4.400     4.400     1.100 peak 15192 weight  0.10000E+01 volume  0.11033E+02 ppm1      3.572 ppm2      1.474
ASSI {15402}
   (( segid "BrD " and resid 82   and name HB2 ))
   (  segid "BrD " and resid 99   and name HB% )
      3.000     3.200     3.200 peak 15402 weight  0.10000E+01 volume  0.10881E+03 ppm1      3.572 ppm2      2.206
ASSI {15412}
   (( segid "BrD " and resid 82   and name HB1 ))
   (  segid "BrD " and resid 99   and name HB% )
      2.900     2.100     2.100 peak 15412 weight  0.10000E+01 volume  0.12753E+03 ppm1      3.672 ppm2      2.206
ASSI {15552}
   (( segid "BrD " and resid 82   and name HB2 ))
   (( segid "BrD " and resid 103  and name HB2 ))
      3.700     3.400     1.800 peak 15552 weight  0.10000E+01 volume  0.31328E+02 ppm1      3.573 ppm2      1.897
ASSI {15592}
   (( segid "BrD " and resid 107  and name HB1 ))
   (( segid "BrD " and resid 103  and name HG2 ))
      3.100     2.400     2.400 peak 15592 weight  0.10000E+01 volume  0.86957E+02 ppm1      3.670 ppm2      2.540
ASSI {15712}
   (( segid "BrD " and resid 107  and name HB1 ))
   (  segid "BrD " and resid 107  and name HD% )
      2.200     1.200     1.200 peak 15712 weight  0.10000E+01 volume  0.63746E+03 ppm1      3.673 ppm2      7.827
ASSI {15812}
   (( segid "BrD " and resid 15   and name HA  ))
   (( segid "BrD " and resid 18   and name HA  ))
      3.300     2.700     2.200 peak 15812 weight  0.10000E+01 volume  0.67333E+02 ppm1      4.606 ppm2      3.900
ASSI {15882}
   (( segid "BrD " and resid 15   and name HB1 ))
   (  segid "BrD " and resid 63   and name HD1%)
      4.000     4.000     1.500 peak 15882 weight  0.10000E+01 volume  0.19033E+02 ppm1      3.815 ppm2      1.652
ASSI {15932}
   (( segid "BrD " and resid 82   and name HB1 ))
   (( segid "BrD " and resid 107  and name HZ  ))
      2.600     1.700     1.700 peak 15932 weight  0.10000E+01 volume  0.26167E+03 ppm1      3.670 ppm2      6.022
ASSI {16052}
   (( segid "BrD " and resid 68   and name HA  ))
   (( segid "BrD " and resid 73   and name HG  ))
      4.000     4.000     1.500 peak 16052 weight  0.10000E+01 volume  0.30921E+02 ppm1      5.148 ppm2      2.367
ASSI {16062}
   (( segid "BrD " and resid 68   and name HB2 ))
   (  segid "BrD " and resid 74   and name HD% )
      3.600     3.200     1.900 peak 16062 weight  0.10000E+01 volume  0.38285E+02 ppm1      3.522 ppm2      6.998
ASSI {16112}
   (( segid "BrD " and resid 68   and name HB1 ))
   (( segid "BrD " and resid 62   and name HD1 ))
      4.500     4.500     1.000 peak 16112 weight  0.10000E+01 volume  0.90000E+01 ppm1      3.669 ppm2      3.148
ASSI {16122}
   (( segid "BrD " and resid 68   and name HB2 ))
   (( segid "BrD " and resid 62   and name HD1 ))
      3.500     3.100     2.000 peak 16122 weight  0.10000E+01 volume  0.43825E+02 ppm1      3.522 ppm2      3.149
ASSI {16132}
   (( segid "BrD " and resid 68   and name HB1 ))
   (( segid "BrD " and resid 63   and name HB1 ))
      3.600     3.200     1.900 peak 16132 weight  0.10000E+01 volume  0.35724E+02 ppm1      3.669 ppm2      2.883
ASSI {16152}
   (( segid "BrD " and resid 68   and name HB2 ))
   (( segid "BrD " and resid 63   and name HB1 ))
      3.500     3.100     2.000 peak 16152 weight  0.10000E+01 volume  0.44106E+02 ppm1      3.522 ppm2      2.884
ASSI {16162}
   (( segid "BrD " and resid 68   and name HB2 ))
   (( segid "BrD " and resid 62   and name HB1 ))
      4.100     4.100     1.400 peak 16162 weight  0.10000E+01 volume  0.16622E+02 ppm1      3.522 ppm2      2.605
ASSI {16212}
   (( segid "BrD " and resid 88   and name HA  ))
   (  segid "BrD " and resid 49   and name HG2%)
      3.200     2.600     2.300 peak 16212 weight  0.10000E+01 volume  0.71276E+02 ppm1      4.999 ppm2      1.571
ASSI {16312}
   (( segid "BrD " and resid 88   and name HB1 ))
   (  segid "BrD " and resid 95   and name HD% )
      3.500     3.100     2.000 peak 16312 weight  0.10000E+01 volume  0.47079E+02 ppm1      3.524 ppm2      7.496
ASSI {16382}
   (( segid "BrD " and resid 19   and name HE1 ))
   (  segid "BrD " and resid 63   and name HD2%)
      3.500     3.100     2.000 peak 16382 weight  0.10000E+01 volume  0.45471E+02 ppm1      3.522 ppm2      1.495
ASSI {16422}
   (( segid "BrD " and resid 66   and name HD2 ))
   (  segid "BrD " and resid 69   and name HG1%)
      4.900     4.900     0.600 peak 16422 weight  0.10000E+01 volume  0.59473E+01 ppm1      3.621 ppm2      1.562
ASSI {16432}
   (( segid "BrD " and resid 66   and name HD2 ))
   (  segid "BrD " and resid 63   and name HD1%)
      4.700     4.700     0.800 peak 16432 weight  0.10000E+01 volume  0.72449E+01 ppm1      3.620 ppm2      1.645
ASSI {16492}
   (( segid "BrD " and resid 96   and name HA  ))
   (( segid "BrD " and resid 86   and name HA  ))
      2.200     1.200     1.200 peak 16492 weight  0.10000E+01 volume  0.78759E+03 ppm1      4.409 ppm2      4.802
ASSI {16502}
   (( segid "BrD " and resid 96   and name HA  ))
   (( segid "BrD " and resid 86   and name HG2 ))
      4.100     4.100     1.400 peak 16502 weight  0.10000E+01 volume  0.17647E+02 ppm1      4.409 ppm2      0.758
ASSI {16612}
   (( segid "BrD " and resid 96   and name HB2 ))
   (  segid "BrD " and resid 96   and name HE% )
      2.400     2.900     2.100 peak 16612 weight  0.10000E+01 volume  0.47985E+02 ppm1      3.134 ppm2      7.633
ASSI {16662}
   (( segid "BrD " and resid 96   and name HB1 ))
   (  segid "BrD " and resid 99   and name HB% )
      4.200     4.200     1.300 peak 16662 weight  0.10000E+01 volume  0.14266E+02 ppm1      4.008 ppm2      2.227
ASSI {16672}
   (( segid "BrD " and resid 96   and name HB2 ))
   (  segid "BrD " and resid 99   and name HB% )
      4.200     4.200     1.300 peak 16672 weight  0.10000E+01 volume  0.13986E+02 ppm1      3.125 ppm2      2.209
ASSI {16682}
   (( segid "BrD " and resid 52   and name HA  ))
   (( segid "BrD " and resid 53   and name HG1 ))
      4.300     4.300     1.200 peak 16682 weight  0.10000E+01 volume  0.11894E+02 ppm1      5.589 ppm2      2.819
OR {16682}
   (( segid "BrD " and resid 52   and name HA  ))
   (( segid "BrD " and resid 53   and name HB1 ))
ASSI {16792}
   (( segid "BrD " and resid 95   and name HB2 ))
   (( segid "BrD " and resid 85   and name HA  ))
      2.700     1.800     1.800 peak 16792 weight  0.10000E+01 volume  0.22670E+03 ppm1      3.375 ppm2      4.995
ASSI {16842}
   (( segid "BrD " and resid 15   and name HB2 ))
   (( segid "BrD " and resid 15   and name HA  ))
      2.200     1.200     1.200 peak 16842 weight  0.10000E+01 volume  0.62256E+03 ppm1      3.677 ppm2      4.618
ASSI {16882}
   (( segid "BrD " and resid 106  and name HA  ))
   (  segid "BrD " and resid 82   and name HE% )
      4.100     4.100     1.400 peak 16882 weight  0.10000E+01 volume  0.17840E+02 ppm1      4.557 ppm2      7.039
OR {16882}
   (( segid "BrD " and resid 106  and name HA  ))
   (( segid "BrD " and resid 82   and name HZ  ))
ASSI {16892}
   (( segid "BrD " and resid 106  and name HA  ))
   (  segid "BrD " and resid 106  and name HD% )
      2.200     1.200     1.200 peak 16892 weight  0.10000E+01 volume  0.63095E+03 ppm1      4.556 ppm2      7.511
ASSI {16902}
   (( segid "BrD " and resid 106  and name HA  ))
   (  segid "BrD " and resid 106  and name HE% )
      3.000     2.200     2.200 peak 16902 weight  0.10000E+01 volume  0.10621E+03 ppm1      4.556 ppm2      7.634
ASSI {16932}
   (( segid "BrD " and resid 57   and name HA  ))
   (( segid "BrD " and resid 36   and name HA  ))
      5.500     5.500     0.000 peak 16932 weight  0.10000E+01 volume  0.15155E+01 ppm1      4.804 ppm2      5.444
ASSI {16972}
   (( segid "BrD " and resid 106  and name HB2 ))
   (  segid "BrD " and resid 82   and name HE% )
      3.000     2.200     2.200 peak 16972 weight  0.10000E+01 volume  0.99455E+02 ppm1      3.676 ppm2      7.053
ASSI {17032}
   (( segid "BrD " and resid 62   and name HA  ))
   (( segid "BrD " and resid 67   and name HB1 ))
      2.400     1.400     1.400 peak 17032 weight  0.10000E+01 volume  0.47084E+03 ppm1      4.462 ppm2      3.576
ASSI {17072}
   (( segid "BrD " and resid 95   and name HA  ))
   (( segid "BrD " and resid 32   and name HN2 ))
      2.800     2.000     2.000 peak 17072 weight  0.10000E+01 volume  0.16966E+03 ppm1      4.462 ppm2      7.790
ASSI {17192}
   (( segid "BrD " and resid 20   and name HA  ))
   (( segid "BrD " and resid 23   and name HG2 ))
      2.400     1.400     1.400 peak 17192 weight  0.10000E+01 volume  0.43323E+03 ppm1      4.903 ppm2      3.069
ASSI {17342}
   (( segid "BrD " and resid 97   and name HA  ))
   (  segid "BrD " and resid 96   and name HD% )
      2.800     2.000     2.000 peak 17342 weight  0.10000E+01 volume  0.15398E+03 ppm1      4.807 ppm2      7.719
ASSI {17352}
   (( segid "BrD " and resid 34   and name HB2 ))
   (  segid "BrD " and resid 102  and name HD1%)
      3.900     3.800     1.600 peak 17352 weight  0.10000E+01 volume  0.22025E+02 ppm1      3.127 ppm2      1.319
OR {17352}
   (( segid "BrD " and resid 34   and name HB2 ))
   (  segid "BrD " and resid 102  and name HD2%)
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ASSI (17372)
  (( segid "BrD " and resid 34   and name HB1 ))
  ( segid "BrD " and resid 102  and name HD1%)
    4.300     4.300     1.200 peak 17372 weight  0.10000E+01 volume  0.12013E+02 ppm1     4.114 ppm2     1.317
OR (17372)
  (( segid "BrD " and resid 34   and name HB1 ))
  ( segid "BrD " and resid 102  and name HD2%)
ASSI (17452)
  (( segid "BrD " and resid 34   and name HB2 ))
  ( segid "BrD " and resid 34   and name HE% )
    3.800     3.600     1.700 peak 17452 weight  0.10000E+01 volume  0.24806E+02 ppm1     3.122 ppm2     7.774
ASSI (17502)
  (( segid "BrD " and resid 34   and name HA  ))
  (( segid "BrD " and resid 35   and name HA  ))
    4.600     4.600     0.900 peak 17502 weight  0.10000E+01 volume  0.81169E+01 ppm1     5.544 ppm2     4.907
ASSI (17562)
  ( segid "BrD " and resid 81   and name HG2%)
  (( segid "BrD " and resid 34   and name HZ  ))
    3.500     3.100     2.000 peak 17562 weight  0.10000E+01 volume  0.45996E+02 ppm1     0.759 ppm2     7.903
ASSI (17572)
  ( segid "BrD " and resid 81   and name HG2%)
  ( segid "BrD " and resid 34   and name HD% )
    2.500     1.600     1.600 peak 17572 weight  0.10000E+01 volume  0.32265E+03 ppm1     0.761 ppm2     7.706
ASSI (17632)
  ( segid "BrD " and resid 81   and name HG2%)
  ( segid "BrD " and resid 82   and name HD% )
    2.300     1.300     1.300 peak 17632 weight  0.10000E+01 volume  0.48682E+03 ppm1     0.763 ppm2     7.263
ASSI (17642)
  ( segid "BrD " and resid 81   and name HG2%)
  ( segid "BrD " and resid 82   and name HE% )
    2.800     2.000     2.000 peak 17642 weight  0.10000E+01 volume  0.15950E+03 ppm1     0.760 ppm2     7.063
ASSI (17712)
  (( segid "BrD " and resid 33   and name HG1 ))
  (( segid "BrD " and resid 95   and name HA  ))
    3.000     2.200     2.200 peak 17712 weight  0.10000E+01 volume  0.11633E+03 ppm1     0.859 ppm2     4.452
ASSI (17732)
  (( segid "BrD " and resid 33   and name HG1 ))
  (( segid "BrD " and resid 98   and name HB1 ))
    3.400     2.900     2.100 peak 17732 weight  0.10000E+01 volume  0.51004E+02 ppm1     0.859 ppm2     4.020
ASSI (17742)
  (( segid "BrD " and resid 33   and name HG1 ))
  (( segid "BrD " and resid 98   and name HB2 ))
    3.100     2.400     2.400 peak 17742 weight  0.10000E+01 volume  0.94735E+02 ppm1     0.859 ppm2     3.654
ASSI (17762)
  (( segid "BrD " and resid 33   and name HG2 ))
  (( segid "BrD " and resid 95   and name HA  ))
    3.400     2.900     2.100 peak 17762 weight  0.10000E+01 volume  0.53516E+02 ppm1    -0.324 ppm2     4.444
ASSI (17782)
  (( segid "BrD " and resid 33   and name HD1 ))
  ( segid "BrD " and resid 31   and name HB% )
    3.500     3.100     2.000 peak 17782 weight  0.10000E+01 volume  0.42246E+02 ppm1     2.782 ppm2     2.304
ASSI (17902)
  (( segid "BrD " and resid 33   and name HD2 ))
  ( segid "BrD " and resid 34   and name HD% )
    3.900     3.800     1.600 peak 17902 weight  0.10000E+01 volume  0.21155E+02 ppm1     2.190 ppm2     7.707
ASSI (17952)
  (( segid "BrD " and resid 33   and name HB1 ))
  (( segid "BrD " and resid 95   and name HA  ))
    3.800     3.600     1.700 peak 17952 weight  0.10000E+01 volume  0.26579E+02 ppm1     1.055 ppm2     4.443
ASSI (17962)
  (( segid "BrD " and resid 33   and name HB2 ))
  (( segid "BrD " and resid 95   and name HA  ))
    3.900     3.800     1.600 peak 17962 weight  0.10000E+01 volume  0.32889E+02 ppm1    -0.176 ppm2     4.444
ASSI (17982)
  (( segid "BrD " and resid 33   and name HB2 ))
  ( segid "BrD " and resid 34   and name HD% )
    3.700     3.400     1.800 peak 17982 weight  0.10000E+01 volume  0.30273E+02 ppm1    -0.174 ppm2     7.699
ASSI (18012)
  (( segid "BrD " and resid 75   and name HG1 ))
  (( segid "BrD " and resid 71   and name HA  ))
    3.200     2.600     2.300 peak 18012 weight  0.10000E+01 volume  0.74474E+02 ppm1     3.524 ppm2     4.662
ASSI (18052)
  (( segid "BrD " and resid 59   and name HG1 ))
  (( segid "BrD " and resid 59   and name HB2 ))
    2.600     1.700     1.700 peak 18052 weight  0.10000E+01 volume  0.28930E+03 ppm1     3.227 ppm2     2.462
OR (18052)
  (( segid "BrD " and resid 59   and name HG2 ))
  (( segid "BrD " and resid 59   and name HB2 ))
ASSI (18102)
  (( segid "BrD " and resid 75   and name HG2 ))
  ( segid "BrD " and resid 115  and name HD1%)
    4.400     4.400     1.100 peak 18102 weight  0.10000E+01 volume  0.10857E+02 ppm1     3.226 ppm2     1.327
ASSI (18112)
  (( segid "BrD " and resid 59   and name HG2 ))
  ( segid "BrD " and resid 22   and name HD1%)
    4.100     4.100     1.400 peak 18112 weight  0.10000E+01 volume  0.16621E+02 ppm1     3.226 ppm2     1.661
OR (18112)
  (( segid "BrD " and resid 59   and name HG1 ))
  ( segid "BrD " and resid 22   and name HD1%)
ASSI (18122)
  (( segid "BrD " and resid 75   and name HG1 ))
  (( segid "BrD " and resid 115  and name HB1 ))
    3.500     3.100     2.000 peak 18122 weight  0.10000E+01 volume  0.47142E+02 ppm1     3.522 ppm2     2.165
ASSI (18142)
  (( segid "BrD " and resid 75   and name HG1 ))
  ( segid "BrD " and resid 113  and name HB% )
    3.900     3.800     1.600 peak 18142 weight  0.10000E+01 volume  0.23045E+02 ppm1     3.523 ppm2     1.996
ASSI (18282)
  ( segid "BrD " and resid 35   and name HE% )
  (( segid "BrD " and resid 60   and name HB1 ))
    2.800     2.000     2.000 peak 18282 weight  0.10000E+01 volume  0.18338E+03 ppm1     2.782 ppm2     4.972
ASSI (18302)
  ( segid "BrD " and resid 35   and name HE% )
  (( segid "BrD " and resid 59   and name HG2 ))
    3.400     2.900     2.100 peak 18302 weight  0.10000E+01 volume  0.50813E+02 ppm1     2.782 ppm2     3.268
OR (18302)
  ( segid "BrD " and resid 35   and name HE% )
  (( segid "BrD " and resid 59   and name HG1 ))
ASSI (18312)
  ( segid "BrD " and resid 35   and name HE% )
  (( segid "BrD " and resid 34   and name HB2 ))
    3.000     2.200     2.200 peak 18312 weight  0.10000E+01 volume  0.11214E+03 ppm1     2.782 ppm2     3.101
ASSI (18352)
  ( segid "BrD " and resid 35   and name HE% )
  ( segid "BrD " and resid 56   and name HD1%)
    2.800     2.000     2.000 peak 18352 weight  0.10000E+01 volume  0.15609E+03 ppm1     2.782 ppm2     1.539
ASSI (18362)
  ( segid "BrD " and resid 35   and name HE% )
  (( segid "BrD " and resid 57   and name HB1 ))
    2.400     1.400     1.400 peak 18362 weight  0.10000E+01 volume  0.41055E+03 ppm1     2.782 ppm2     2.938
ASSI (18382)
  ( segid "BrD " and resid 35   and name HE% )
  (( segid "BrD " and resid 26   and name HB1 ))
    2.500     1.600     1.600 peak 18382 weight  0.10000E+01 volume  0.29206E+03 ppm1     2.781 ppm2     2.460
ASSI (18492)
  (( segid "BrD " and resid 59   and name HG1 ))
  ( segid "BrD " and resid 74   and name HE% )
    5.000     5.000     0.500 peak 18492 weight  0.10000E+01 volume  0.50782E+01 ppm1     3.226 ppm2     7.552
OR (18492)
  (( segid "BrD " and resid 59   and name HG2 ))
  ( segid "BrD " and resid 74   and name HE% )
ASSI (18542)
  ( segid "BrD " and resid 75   and name HE% )
  (( segid "BrD " and resid 17   and name HB  ))
    3.000     2.200     2.200 peak 18542 weight  0.10000E+01 volume  0.10304E+03 ppm1     2.634 ppm2     4.826
ASSI (18642)
  ( segid "BrD " and resid 75   and name HE% )
  (( segid "BrD " and resid 110  and name HA  ))
    3.400     2.900     2.100 peak 18642 weight  0.10000E+01 volume  0.51911E+02 ppm1     2.634 ppm2     4.427
ASSI (18662)
  ( segid "BrD " and resid 75   and name HE% )
  (( segid "BrD " and resid 74   and name HB1 ))
    2.900     2.100     2.100 peak 18662 weight  0.10000E+01 volume  0.13576E+03 ppm1     2.634 ppm2     3.597
ASSI (18682)
  ( segid "BrD " and resid 75   and name HE% )
  (( segid "BrD " and resid 74   and name HB2 ))
    3.000     2.200     2.200 peak 18682 weight  0.10000E+01 volume  0.11929E+03 ppm1     2.634 ppm2     3.003
ASSI (18722)
  ( segid "BrD " and resid 75   and name HE% )
  (( segid "BrD " and resid 75   and name HB1 ))
    3.700     3.400     1.800 peak 18722 weight  0.10000E+01 volume  0.33115E+02 ppm1     2.634 ppm2     2.906
ASSI (18732)
  ( segid "BrD " and resid 75   and name HE% )
  (( segid "BrD " and resid 75   and name HB2 ))
    2.100     2.100     2.400 peak 18732 weight  0.10000E+01 volume  0.10446E+04 ppm1     2.634 ppm2     2.824
ASSI (18742)
  ( segid "BrD " and resid 75   and name HE% )
  ( segid "BrD " and resid 78   and name HD2%)
    4.900     4.900     0.600 peak 18742 weight  0.10000E+01 volume  0.60943E+01 ppm1     2.634 ppm2     0.676
ASSI (18772)
  ( segid "BrD " and resid 75   and name HE% )
  ( segid "BrD " and resid 14   and name HD1%)
    2.600     1.700     1.700 peak 18772 weight  0.10000E+01 volume  0.27797E+03 ppm1     2.634 ppm2     1.425
OR (18772)
  ( segid "BrD " and resid 75   and name HE% )
  ( segid "BrD " and resid 14   and name HD2%)
ASSI (18782)
  ( segid "BrD " and resid 75   and name HE% )
  ( segid "BrD " and resid 115  and name HD1%)
    2.800     2.000     2.000 peak 18782 weight  0.10000E+01 volume  0.15408E+03 ppm1     2.634 ppm2     1.327
ASSI (18812)
  ( segid "BrD " and resid 75   and name HE% )
  (( segid "BrD " and resid 116  and name HG12))
    3.600     3.200     1.900 peak 18812 weight  0.10000E+01 volume  0.36651E+02 ppm1     2.635 ppm2     1.547
ASSI (18862)
  ( segid "BrD " and resid 75   and name HE% )
  (( segid "BrD " and resid 116  and name HG11))
    4.600     4.600     0.900 peak 18862 weight  0.10000E+01 volume  0.78723E+01 ppm1     2.635 ppm2     1.914
ASSI (18872)
  ( segid "BrD " and resid 75   and name HE% )
  ( segid "BrD " and resid 59   and name HE% )
    3.500     3.100     2.000 peak 18872 weight  0.10000E+01 volume  0.40230E+02 ppm1     2.635 ppm2     1.865
ASSI (18882)
  ( segid "BrD " and resid 75   and name HE% )
  ( segid "BrD " and resid 113  and name HB% )
    2.700     1.800     1.800 peak 18882 weight  0.10000E+01 volume  0.23578E+03 ppm1     2.634 ppm2     1.986
ASSI (18892)
  ( segid "BrD " and resid 75   and name HE% )
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   (( segid "BrD " and resid 18   and name HG  ))
      2.400     1.400     1.400 peak 18892 weight  0.10000E+01 volume  0.37764E+03 ppm1      2.636 ppm2      2.250
ASSI (18902)
   (  segid "BrD " and resid 75   and name HE% )
   (( segid "BrD " and resid 115  and name HB1 ))
      2.500     1.600     1.600 peak 18902 weight  0.10000E+01 volume  0.35880E+03 ppm1      2.635 ppm2      2.199
ASSI (18932)
   (  segid "BrD " and resid 75   and name HE% )
   (( segid "BrD " and resid 14   and name HB1 ))
      3.700     3.400     1.800 peak 18932 weight  0.10000E+01 volume  0.29255E+02 ppm1      2.636 ppm2      2.444
ASSI (18952)
   (( segid "BrD " and resid 57   and name HB2 ))
   (( segid "BrD " and resid 37   and name HD1 ))
      3.200     2.600     2.300 peak 18952 weight  0.10000E+01 volume  0.68763E+02 ppm1      2.847 ppm2      4.289
ASSI (18992)
   (( segid "BrD " and resid 57   and name HB2 ))
   (( segid "BrD " and resid 36   and name HA  ))
      3.700     3.400     1.800 peak 18992 weight  0.10000E+01 volume  0.28694E+02 ppm1      2.842 ppm2      5.444
ASSI (19072)
   (( segid "BrD " and resid 31   and name HA  ))
   (( segid "BrD " and resid 34   and name HZ  ))
      3.100     2.400     2.400 peak 19072 weight  0.10000E+01 volume  0.98899E+02 ppm1      5.001 ppm2      7.893
ASSI (19092)
   (( segid "BrD " and resid 31   and name HA  ))
   (( segid "BrD " and resid 30   and name HA  ))
      2.800     2.000     2.000 peak 19092 weight  0.10000E+01 volume  0.15610E+03 ppm1      5.001 ppm2      5.428
ASSI (19172)
   (( segid "BrD " and resid 43   and name HA  ))
   (  segid "BrD " and resid 88   and name HE% )
      3.300     2.700     2.200 peak 19172 weight  0.10000E+01 volume  0.58224E+02 ppm1      5.547 ppm2      7.417
ASSI (19182)
   (( segid "BrD " and resid 43   and name HA  ))
   (( segid "BrD " and resid 44   and name HG1 ))
      2.900     2.100     2.100 peak 19182 weight  0.10000E+01 volume  0.12258E+03 ppm1      5.544 ppm2      2.735
ASSI (19192)
   (( segid "BrD " and resid 43   and name HA  ))
   (( segid "BrD " and resid 44   and name HG2 ))
      3.100     2.400     2.400 peak 19192 weight  0.10000E+01 volume  0.97301E+02 ppm1      5.544 ppm2      2.646
OR (19192)
   (( segid "BrD " and resid 43   and name HA  ))
   (( segid "BrD " and resid 44   and name HB2 ))
ASSI (19202)
   (( segid "BrD " and resid 43   and name HA  ))
   (  segid "BrD " and resid 38   and name HG2% )
      3.500     3.100     2.000 peak 19202 weight  0.10000E+01 volume  0.42319E+02 ppm1      5.544 ppm2      0.799
ASSI (19212)
   (  segid "BrD " and resid 43   and name HB% )
   (( segid "BrD " and resid 42   and name HG1 ))
      3.600     3.200     1.900 peak 19212 weight  0.10000E+01 volume  0.35927E+02 ppm1      1.697 ppm2      2.898
ASSI (19242)
   (  segid "BrD " and resid 43   and name HB% )
   (  segid "BrD " and resid 50   and name HD1% )
      5.400     5.400     0.100 peak 19242 weight  0.10000E+01 volume  0.31463E+01 ppm1      1.697 ppm2      1.148
ASSI (19272)
   (  segid "BrD " and resid 43   and name HB% )
   (( segid "BrD " and resid 39   and name HG1 ))
      3.300     2.700     2.200 peak 19272 weight  0.10000E+01 volume  0.60793E+02 ppm1      1.697 ppm2      2.032
ASSI (19282)
   (  segid "BrD " and resid 43   and name HB% )
   (( segid "BrD " and resid 38   and name HB  ))
      3.000     2.200     2.200 peak 19282 weight  0.10000E+01 volume  0.12013E+03 ppm1      1.697 ppm2      1.790
ASSI (19312)
   (  segid "BrD " and resid 31   and name HB% )
   (  segid "BrD " and resid 25   and name HG1% )
      3.200     2.600     2.300 peak 19312 weight  0.10000E+01 volume  0.68019E+02 ppm1      2.289 ppm2      1.832
ASSI (19352)
   (  segid "BrD " and resid 31   and name HB% )
   (( segid "BrD " and resid 35   and name HB1 ))
      3.400     2.900     2.100 peak 19352 weight  0.10000E+01 volume  0.48169E+02 ppm1      2.289 ppm2      2.841
ASSI (19362)
   (  segid "BrD " and resid 31   and name HB% )
   (( segid "BrD " and resid 28   and name HB1 ))
      2.400     1.400     1.400 peak 19362 weight  0.10000E+01 volume  0.37768E+03 ppm1      2.289 ppm2      3.581
ASSI (19372)
   (  segid "BrD " and resid 31   and name HB% )
   (( segid "BrD " and resid 35   and name HG1 ))
      2.500     1.600     1.600 peak 19372 weight  0.10000E+01 volume  0.30400E+03 ppm1      2.289 ppm2      3.427
ASSI (19382)
   (  segid "BrD " and resid 31   and name HB% )
   (( segid "BrD " and resid 34   and name HB2 ))
      4.200     4.200     1.300 peak 19382 weight  0.10000E+01 volume  0.14651E+02 ppm1      2.289 ppm2      3.134
ASSI (19392)
   (  segid "BrD " and resid 31   and name HB% )
   (( segid "BrD " and resid 28   and name HA  ))
      3.100     2.400     2.400 peak 19392 weight  0.10000E+01 volume  0.87183E+02 ppm1      2.289 ppm2      4.582
ASSI (19422)
   (  segid "BrD " and resid 31   and name HB% )
   (  segid "BrD " and resid 34   and name HE% )
      3.500     3.100     2.000 peak 19422 weight  0.10000E+01 volume  0.44223E+02 ppm1      2.289 ppm2      7.803
ASSI (19482)
   (  segid "BrD " and resid 76   and name HB% )
   (( segid "BrD " and resid 79   and name HB2 ))
      3.300     2.700     2.200 peak 19482 weight  0.10000E+01 volume  0.66817E+02 ppm1      2.092 ppm2      2.662
ASSI (19492)
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   (  segid "BrD " and resid 76   and name HB% )
   (( segid "BrD " and resid 80   and name HB2 ))
      2.800     2.000     2.000 peak 19492 weight  0.10000E+01 volume  0.15977E+03 ppm1      2.092 ppm2      2.564
OR (19492)
   (  segid "BrD " and resid 76   and name HB% )
   (( segid "BrD " and resid 80   and name HB1 ))
ASSI (19502)
   (  segid "BrD " and resid 76   and name HB% )
   (( segid "BrD " and resid 80   and name HB2 ))
      2.700     1.800     1.800 peak 19502 weight  0.10000E+01 volume  0.21436E+03 ppm1      2.092 ppm2      2.507
ASSI (19522)
   (  segid "BrD " and resid 76   and name HB% )
   (( segid "BrD " and resid 77   and name HA  ))
      2.800     2.000     2.000 peak 19522 weight  0.10000E+01 volume  0.15327E+03 ppm1      2.092 ppm2      4.963
ASSI (19552)
   (  segid "BrD " and resid 76   and name HB% )
   (( segid "BrD " and resid 51   and name HB2 ))
      2.500     1.600     1.600 peak 19552 weight  0.10000E+01 volume  0.32487E+03 ppm1      2.092 ppm2      1.783
OR (19552)
   (  segid "BrD " and resid 76   and name HB% )
   (( segid "BrD " and resid 51   and name HG2 ))
ASSI (19572)
   (  segid "BrD " and resid 76   and name HB% )
   (  segid "BrD " and resid 116  and name HG2% )
      3.600     3.200     1.900 peak 19572 weight  0.10000E+01 volume  0.35020E+02 ppm1      2.092 ppm2      1.432
ASSI (19582)
   (  segid "BrD " and resid 73   and name HD2% )
   (( segid "BrD " and resid 68   and name HA  ))
      2.800     2.000     2.000 peak 19582 weight  0.10000E+01 volume  0.14681E+03 ppm1      1.500 ppm2      5.143
ASSI (19632)
   (( segid "BrD " and resid 76   and name HA  ))
   (( segid "BrD " and resid 80   and name HG1 ))
      3.100     2.400     2.400 peak 19632 weight  0.10000E+01 volume  0.95067E+02 ppm1      4.656 ppm2      2.327
ASSI (19642)
   (  segid "BrD " and resid 99   and name HB% )
   (( segid "BrD " and resid 34   and name HZ  ))
      2.200     2.200     2.200 peak 19642 weight  0.10000E+01 volume  0.65240E+03 ppm1      2.190 ppm2      7.903
ASSI (19652)
   (  segid "BrD " and resid 99   and name HB% )
   (  segid "BrD " and resid 34   and name HE% )
      2.300     1.300     1.300 peak 19652 weight  0.10000E+01 volume  0.50164E+03 ppm1      2.190 ppm2      7.781
ASSI (19672)
   (  segid "BrD " and resid 99   and name HB% )
   (  segid "BrD " and resid 82   and name HD% )
      2.500     1.600     1.600 peak 19672 weight  0.10000E+01 volume  0.36039E+03 ppm1      2.190 ppm2      7.259
ASSI (19692)
   (  segid "BrD " and resid 99   and name HB% )
   (( segid "BrD " and resid 85   and name HA  ))
      3.100     2.400     2.400 peak 19692 weight  0.10000E+01 volume  0.92786E+02 ppm1      2.190 ppm2      5.005
ASSI (19702)
   (  segid "BrD " and resid 99   and name HB% )
   (( segid "BrD " and resid 100  and name HA  ))
      3.000     2.200     2.200 peak 19702 weight  0.10000E+01 volume  0.10441E+03 ppm1      2.190 ppm2      4.948
ASSI (19752)
   (  segid "BrD " and resid 99   and name HB% )
   (( segid "BrD " and resid 103  and name HG1 ))
      3.000     2.200     2.200 peak 19752 weight  0.10000E+01 volume  0.10256E+03 ppm1      2.190 ppm2      2.613
ASSI (19772)
   (  segid "BrD " and resid 76   and name HB% )
   (( segid "BrD " and resid 79   and name HB1 ))
      3.500     3.100     2.000 peak 19772 weight  0.10000E+01 volume  0.45000E+02 ppm1      2.092 ppm2      2.784
ASSI (19792)
   (( segid "BrD " and resid 99   and name HA  ))
   (( segid "BrD " and resid 34   and name HZ  ))
      2.600     1.700     1.700 peak 19792 weight  0.10000E+01 volume  0.26558E+03 ppm1      4.459 ppm2      7.901
ASSI (19802)
   (( segid "BrD " and resid 99   and name HA  ))
   (  segid "BrD " and resid 34   and name HE% )
      2.700     1.800     1.800 peak 19802 weight  0.10000E+01 volume  0.21467E+03 ppm1      4.459 ppm2      7.771
ASSI (19812)
   (( segid "BrD " and resid 99   and name HA  ))
   (  segid "BrD " and resid 82   and name HE% )
      3.200     2.600     2.300 peak 19812 weight  0.10000E+01 volume  0.71395E+02 ppm1      4.457 ppm2      7.073
ASSI (19822)
   (( segid "BrD " and resid 99   and name HA  ))
   (  segid "BrD " and resid 82   and name HD% )
      2.800     2.000     2.000 peak 19822 weight  0.10000E+01 volume  0.15492E+03 ppm1      4.459 ppm2      7.259
ASSI (19832)
   (( segid "BrD " and resid 99   and name HA  ))
   (( segid "BrD " and resid 100  and name HA  ))
      2.800     2.000     2.000 peak 19832 weight  0.10000E+01 volume  0.16591E+03 ppm1      4.458 ppm2      4.950
ASSI (19842)
   (( segid "BrD " and resid 99   and name HA  ))
   (( segid "BrD " and resid 103  and name HB2 ))
      2.600     1.700     1.700 peak 19842 weight  0.10000E+01 volume  0.24667E+03 ppm1      4.458 ppm2      1.922
ASSI (19882)
   (( segid "BrD " and resid 113  and name HA  ))
   (  segid "BrD " and resid 110  and name HG2% )
      3.600     3.200     1.900 peak 19882 weight  0.10000E+01 volume  0.35803E+02 ppm1      4.903 ppm2      1.222
ASSI (19902)
   (( segid "BrD " and resid 113  and name HA  ))
   (( segid "BrD " and resid 112  and name HB1 ))
      3.400     2.900     2.100 peak 19902 weight  0.10000E+01 volume  0.48798E+02 ppm1      4.903 ppm2      3.670
ASSI (19912)
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   (( segid "BrD " and resid 113  and name HA  ))
   (( segid "BrD " and resid 110  and name HA  ))
    3.500     3.100     2.000 peak 19912 weight  0.10000E+01 volume  0.44605E+02 ppm1      4.903 ppm2      4.419
ASSI (19922)
   (( segid "BrD " and resid 113  and name HA  ))
   (( segid "BrD " and resid 14   and name HA  ))
    3.100     2.400     2.400 peak 19922 weight  0.10000E+01 volume  0.84488E+02 ppm1      4.903 ppm2      4.663
ASSI (19962)
   (( segid "BrD " and resid 113  and name HA  ))
   ( segid "BrD " and resid 115  and name HD1%)
    4.000     4.000     1.500 peak 19962 weight  0.10000E+01 volume  0.18572E+02 ppm1      4.899 ppm2      1.313
ASSI (19992)
   ( segid "BrD " and resid 113  and name HB% )
   (( segid "BrD " and resid 14   and name HB1 ))
    3.300     2.700     2.200 peak 19992 weight  0.10000E+01 volume  0.60405E+02 ppm1      1.991 ppm2      2.442
ASSI (20032)
   ( segid "BrD " and resid 113  and name HB% )
   (( segid "BrD " and resid 14   and name HG  ))
    2.100     2.100     2.400 peak 20032 weight  0.10000E+01 volume  0.86636E+03 ppm1      1.994 ppm2      2.059
ASSI (20042)
   ( segid "BrD " and resid 113  and name HB% )
   ( segid "BrD " and resid 18   and name HD2%)
    4.200     4.200     1.300 peak 20042 weight  0.10000E+01 volume  0.14101E+02 ppm1      1.993 ppm2      0.408
ASSI (20052)
   ( segid "BrD " and resid 113  and name HB% )
   ( segid "BrD " and resid 115  and name HD1%)
    2.400     1.400     1.400 peak 20052 weight  0.10000E+01 volume  0.47259E+03 ppm1      1.993 ppm2      1.319
ASSI (20072)
   (( segid "BrD " and resid 110  and name HA  ))
   ( segid "BrD " and resid 115  and name HD1%)
    2.800     1.800     1.800 peak 20072 weight  0.10000E+01 volume  0.33630E+03 ppm1      4.409 ppm2      1.319
ASSI (20192)
   (( segid "BrD " and resid 17   and name HB  ))
   ( segid "BrD " and resid 115  and name HD1%)
    3.200     2.600     2.300 peak 20192 weight  0.10000E+01 volume  0.76060E+02 ppm1      4.854 ppm2      1.327
ASSI (20212)
   (( segid "BrD " and resid 17   and name HA  ))
   ( segid "BrD " and resid 21   and name HD1%)
    4.600     4.600     0.900 peak 20212 weight  0.10000E+01 volume  0.88717E+01 ppm1      4.542 ppm2      1.224
ASSI (20242)
   ( segid "BrD " and resid 17   and name HG2%)
   ( segid "BrD " and resid 75   and name HE% )
    2.600     1.700     1.700 peak 20242 weight  0.10000E+01 volume  0.27619E+03 ppm1      1.747 ppm2      2.619
ASSI (20252)
   ( segid "BrD " and resid 17   and name HG2%)
   (( segid "BrD " and resid 21   and name HB  ))
    3.000     2.200     2.200 peak 20252 weight  0.10000E+01 volume  0.10098E+03 ppm1      1.747 ppm2      2.507
ASSI (20272)
   ( segid "BrD " and resid 17   and name HG2%)
   (( segid "BrD " and resid 115  and name HB1 ))
    3.500     3.100     2.000 peak 20272 weight  0.10000E+01 volume  0.46134E+02 ppm1      1.747 ppm2      2.214
ASSI (20292)
   ( segid "BrD " and resid 17   and name HG2%)
   (( segid "BrD " and resid 109  and name HB2 ))
    2.600     1.700     1.700 peak 20292 weight  0.10000E+01 volume  0.25743E+03 ppm1      1.747 ppm2      2.149
ASSI (20302)
   ( segid "BrD " and resid 17   and name HG2%)
   (( segid "BrD " and resid 18   and name HB2 ))
    4.600     4.600     0.900 peak 20302 weight  0.10000E+01 volume  0.84610E+01 ppm1      1.747 ppm2      0.904
ASSI (20312)
   (( segid "BrD " and resid 41   and name HB  ))
   (( segid "BrD " and resid 39   and name HD1 ))
    3.300     2.700     2.200 peak 20312 weight  0.10000E+01 volume  0.67487E+02 ppm1      4.903 ppm2      2.271
ASSI (20332)
   (( segid "BrD " and resid 41   and name HA  ))
   (( segid "BrD " and resid 44   and name HD2 ))
    3.500     3.100     2.000 peak 20332 weight  0.10000E+01 volume  0.42717E+02 ppm1      4.656 ppm2      4.143
ASSI (20362)
   (( segid "BrD " and resid 41   and name HA  ))
   (( segid "BrD " and resid 44   and name HD1 ))
    2.900     2.100     2.100 peak 20362 weight  0.10000E+01 volume  0.13674E+03 ppm1      4.656 ppm2      4.308
ASSI (20532)
   ( segid "BrD " and resid 41   and name HG2%)
   (( segid "BrD " and resid 42   and name HA  ))
    3.400     2.900     2.100 peak 20532 weight  0.10000E+01 volume  0.51387E+02 ppm1      1.845 ppm2      5.062
ASSI (20542)
   ( segid "BrD " and resid 41   and name HG2%)
   (( segid "BrD " and resid 39   and name HG1 ))
    2.600     1.700     1.700 peak 20542 weight  0.10000E+01 volume  0.28354E+03 ppm1      1.844 ppm2      2.019
ASSI (20562)
   ( segid "BrD " and resid 41   and name HG2%)
   (( segid "BrD " and resid 39   and name HD1 ))
    2.900     2.100     2.100 peak 20562 weight  0.10000E+01 volume  0.13596E+03 ppm1      1.844 ppm2      2.296
ASSI (20572)
   ( segid "BrD " and resid 41   and name HG2%)
   (( segid "BrD " and resid 39   and name HB1 ))
    3.200     2.600     2.300 peak 20572 weight  0.10000E+01 volume  0.75085E+02 ppm1      1.845 ppm2      2.466
ASSI (20592)
   (( segid "BrD " and resid 112  and name HG2 ))
   (( segid "BrD " and resid 112  and name HA  ))
    2.400     1.400     1.400 peak 20592 weight  0.10000E+01 volume  0.44748E+03 ppm1      2.832 ppm2      4.585
ASSI (20712)
   (( segid "BrD " and resid 67   and name HA  ))
   (( segid "BrD " and resid 68   and name HA  ))
    2.800     2.000     2.000 peak 20712 weight  0.10000E+01 volume  0.17530E+03 ppm1      4.656 ppm2      5.111
ASSI (20802)
   ( segid "BrD " and resid 25   and name HG2%)
   ( segid "BrD " and resid 82   and name HE% )
    2.900     2.100     2.100 peak 20802 weight  0.10000E+01 volume  0.13726E+03 ppm1      1.648 ppm2      7.026
OR (20802)
   ( segid "BrD " and resid 25   and name HG2%)
   (( segid "BrD " and resid 82   and name HZ  ))
ASSI (20812)
   ( segid "BrD " and resid 58   and name HG2%)
   ( segid "BrD " and resid 68   and name HE% )
    3.200     2.600     2.300 peak 20812 weight  0.10000E+01 volume  0.69885E+02 ppm1      1.651 ppm2      7.920
ASSI (20852)
   ( segid "BrD " and resid 25   and name HG2%)
   (( segid "BrD " and resid 31   and name HA  ))
    3.400     2.900     2.100 peak 20852 weight  0.10000E+01 volume  0.55839E+02 ppm1      1.649 ppm2      4.980
ASSI (20862)
   (( segid "BrD " and resid 62   and name HD1 ))
   (( segid "BrD " and resid 62   and name HB2 ))
    2.900     2.100     2.100 peak 20862 weight  0.10000E+01 volume  0.12367E+03 ppm1      3.175 ppm2      1.710
ASSI (20872)
   (( segid "BrD " and resid 62   and name HD2 ))
   (( segid "BrD " and resid 62   and name HB2 ))
    3.000     2.200     2.200 peak 20872 weight  0.10000E+01 volume  0.11189E+03 ppm1      2.633 ppm2      1.711
ASSI (20992)
   (( segid "BrD " and resid 62   and name HB1 ))
   ( segid "BrD " and resid 68   and name HE% )
    3.100     2.400     2.400 peak 20992 weight  0.10000E+01 volume  0.97485E+02 ppm1      2.636 ppm2      7.905
ASSI (21082)
   ( segid "BrD " and resid 83   and name HG2%)
   (( segid "BrD " and resid 87   and name HG2 ))
    3.000     2.200     2.200 peak 21082 weight  0.10000E+01 volume  0.11102E+03 ppm1      1.895 ppm2      2.784
ASSI (21142)
   (( segid "BrD " and resid 83   and name HB  ))
   (( segid "BrD " and resid 80   and name HG1 ))
    3.400     2.900     2.100 peak 21142 weight  0.10000E+01 volume  0.55703E+02 ppm1      4.803 ppm2      2.360
ASSI (21192)
   ( segid "BrD " and resid 83   and name HG2%)
   (( segid "BrD " and resid 87   and name HG1 ))
    2.100     1.100     1.100 peak 21192 weight  0.10000E+01 volume  0.10489E+04 ppm1      1.895 ppm2      3.038
ASSI (21202)
   ( segid "BrD " and resid 83   and name HG2%)
   (( segid "BrD " and resid 87   and name HB2 ))
    3.400     2.900     2.100 peak 21202 weight  0.10000E+01 volume  0.47828E+02 ppm1      1.899 ppm2      2.597
ASSI (21292)
   ( segid "BrD " and resid 25   and name HG1%)
   ( segid "BrD " and resid 106  and name HD% )
    2.500     2.500     2.000 peak 21292 weight  0.10000E+01 volume  0.35912E+03 ppm1      1.795 ppm2      7.515
ASSI (21322)
   ( segid "BrD " and resid 25   and name HG1%)
   ( segid "BrD " and resid 82   and name HE% )
    3.500     3.100     2.000 peak 21322 weight  0.10000E+01 volume  0.43989E+02 ppm1      1.795 ppm2      7.026
OR (21322)
   ( segid "BrD " and resid 25   and name HG1%)
   (( segid "BrD " and resid 82   and name HZ  ))
ASSI (21392)
   (( segid "BrD " and resid 25   and name HB  ))
   ( segid "BrD " and resid 102  and name HD1%)
    3.600     3.200     1.900 peak 21392 weight  0.10000E+01 volume  0.35593E+02 ppm1      2.979 ppm2      1.327
OR (21392)
   (( segid "BrD " and resid 25   and name HB  ))
   ( segid "BrD " and resid 102  and name HD2%)
ASSI (21402)
   (( segid "BrD " and resid 25   and name HB  ))
   ( segid "BrD " and resid 76   and name HD2%)
    4.400     4.400     1.100 peak 21402 weight  0.10000E+01 volume  0.11302E+02 ppm1      2.979 ppm2      0.676
ASSI (21422)
   ( segid "BrD " and resid 25   and name HG1%)
   (( segid "BrD " and resid 102  and name HG  ))
    3.500     3.100     2.000 peak 21422 weight  0.10000E+01 volume  0.43674E+02 ppm1      1.795 ppm2      2.157
ASSI (21452)
   ( segid "BrD " and resid 25   and name HG1%)
   (( segid "BrD " and resid 106  and name HB1 ))
    4.300     4.300     1.200 peak 21452 weight  0.10000E+01 volume  0.11856E+02 ppm1      1.796 ppm2      3.907
ASSI (21462)
   ( segid "BrD " and resid 25   and name HG1%)
   (( segid "BrD " and resid 21   and name HA  ))
    2.700     1.800     1.800 peak 21462 weight  0.10000E+01 volume  0.21023E+03 ppm1      1.797 ppm2      4.369
ASSI (21472)
   ( segid "BrD " and resid 25   and name HG1%)
   (( segid "BrD " and resid 102  and name HA  ))
    3.400     2.900     2.100 peak 21472 weight  0.10000E+01 volume  0.48930E+02 ppm1      1.796 ppm2      4.297
ASSI (21562)
   ( segid "BrD " and resid 81   and name HG2%)
   (( segid "BrD " and resid 82   and name HA  ))
    2.900     2.100     2.100 peak 21562 weight  0.10000E+01 volume  0.12812E+03 ppm1      0.760 ppm2      4.783
ASSI (21582)
   ( segid "BrD " and resid 38   and name HG1%)
   (( segid "BrD " and resid 37   and name HA  ))
    3.300     2.700     2.200 peak 21582 weight  0.10000E+01 volume  0.64039E+02 ppm1      1.056 ppm2      4.859
ASSI (21672)
   ( segid "BrD " and resid 81   and name HG1%)
   ( segid "BrD " and resid 24   and name HD% )
    3.400     2.900     2.100 peak 21672 weight  0.10000E+01 volume  0.52778E+02 ppm1      1.056 ppm2      7.706
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ASSI (21702)
  ( segid "BrD " and resid 38   and name HG2%)
  (( segid "BrD " and resid 41   and name HA  ))
     4.900      4.900      0.600 peak 21702 weight  0.10000E+01 volume  0.56291E+01 ppm1      0.808 ppm2      4.646
ASSI (21732)
  ( segid "BrD " and resid 81   and name HG2%)
  ( segid "BrD " and resid 56   and name HD2%)
     2.600      1.700      1.700 peak 21732 weight  0.10000E+01 volume  0.28103E+03 ppm1      0.760 ppm2      1.238
ASSI (21742)
  ( segid "BrD " and resid 81   and name HG2%)
  ( segid "BrD " and resid 102  and name HD1%)
     3.900      3.800      1.600 peak 21742 weight  0.10000E+01 volume  0.21895E+02 ppm1      0.760 ppm2      1.319
OR (21742)
  ( segid "BrD " and resid 81   and name HG2%)
  ( segid "BrD " and resid 102  and name HD2%)
ASSI (21752)
  ( segid "BrD " and resid 81   and name HG2%)
  (( segid "BrD " and resid 84   and name HB2 ))
     3.000      2.200      2.200 peak 21752 weight  0.10000E+01 volume  0.11571E+03 ppm1      0.763 ppm2      3.296
ASSI (21772)
  (( segid "BrD " and resid 81   and name HB  ))
  ( segid "BrD " and resid 78   and name HD2%)
     3.200      2.600      2.300 peak 21772 weight  0.10000E+01 volume  0.80152E+02 ppm1      2.042 ppm2      0.683
ASSI (21802)
  (( segid "BrD " and resid 81   and name HA  ))
  (( segid "BrD " and resid 80   and name HB1 ))
     3.900      3.800      1.600 peak 21802 weight  0.10000E+01 volume  0.23614E+02 ppm1      3.719 ppm2      2.564
OR (21802)
  (( segid "BrD " and resid 81   and name HA  ))
  (( segid "BrD " and resid 80   and name HB2 ))
ASSI (21812)
  (( segid "BrD " and resid 81   and name HA  ))
  (( segid "BrD " and resid 80   and name HB1 ))
     3.600      3.200      1.900 peak 21812 weight  0.10000E+01 volume  0.37077E+02 ppm1      3.719 ppm2      2.597
ASSI (21902)
  (( segid "BrD " and resid 49   and name HA  ))
  ( segid "BrD " and resid 50   and name HD1%)
     4.100      4.100      1.400 peak 21902 weight  0.10000E+01 volume  0.17504E+02 ppm1      4.656 ppm2      1.140
ASSI (21952)
  ( segid "BrD " and resid 50   and name HD1%)
  (( segid "BrD " and resid 88   and name HB1 ))
     2.400      1.400      1.400 peak 21952 weight  0.10000E+01 volume  0.36864E+03 ppm1      1.155 ppm2      3.535
ASSI (21972)
  ( segid "BrD " and resid 50   and name HD1%)
  (( segid "BrD " and resid 46   and name HA  ))
     4.100      4.100      1.400 peak 21972 weight  0.10000E+01 volume  0.16984E+02 ppm1      1.155 ppm2      4.151
ASSI (22022)
  ( segid "BrD " and resid 50   and name HD1%)
  ( segid "BrD " and resid 88   and name HD% )
     3.100      2.400      2.400 peak 22022 weight  0.10000E+01 volume  0.82494E+02 ppm1      1.155 ppm2      7.606
ASSI (22042)
  (( segid "BrD " and resid 50   and name HB  ))
  (( segid "BrD " and resid 51   and name HB1 ))
     4.800      4.800      0.700 peak 22042 weight  0.10000E+01 volume  0.67010E+01 ppm1      1.797 ppm2      1.966
OR (22042)
  (( segid "BrD " and resid 50   and name HB  ))
  (( segid "BrD " and resid 51   and name HG1 ))
ASSI (22132)
  (( segid "BrD " and resid 50   and name HA  ))
  ( segid "BrD " and resid 49   and name HG2%)
     2.500      1.600      1.600 peak 22132 weight  0.10000E+01 volume  0.30657E+03 ppm1      4.506 ppm2      1.570
ASSI (22142)
  (( segid "BrD " and resid 50   and name HA  ))
  ( segid "BrD " and resid 49   and name HG1%)
     3.800      3.600      1.700 peak 22142 weight  0.10000E+01 volume  0.27941E+02 ppm1      4.506 ppm2      1.646
ASSI (22212)
  ( segid "BrD " and resid 50   and name HG2%)
  (( segid "BrD " and resid 51   and name HB1 ))
     4.000      4.000      1.500 peak 22212 weight  0.10000E+01 volume  0.20287E+02 ppm1      1.007 ppm2      1.954
ASSI (22222)
  (( segid "BrD " and resid 84   and name HA  ))
  ( segid "BrD " and resid 83   and name HG2%)
     4.100      4.100      1.400 peak 22222 weight  0.10000E+01 volume  0.17290E+02 ppm1      4.903 ppm2      1.913
ASSI (22232)
  (( segid "BrD " and resid 84   and name HA  ))
  (( segid "BrD " and resid 87   and name HG1 ))
     3.500      3.100      2.000 peak 22232 weight  0.10000E+01 volume  0.41523E+02 ppm1      4.904 ppm2      3.010
ASSI (22242)
  (( segid "BrD " and resid 84   and name HA  ))
  (( segid "BrD " and resid 88   and name HB1 ))
     3.100      2.400      2.400 peak 22242 weight  0.10000E+01 volume  0.82436E+02 ppm1      4.904 ppm2      3.533
ASSI (22322)
  ( segid "BrD " and resid 69   and name HG1%)
  (( segid "BrD " and resid 66   and name HA  ))
     2.800      2.000      2.000 peak 22322 weight  0.10000E+01 volume  0.17920E+03 ppm1      1.551 ppm2      4.989
ASSI (22332)
  ( segid "BrD " and resid 69   and name HG1%)
  (( segid "BrD " and resid 68   and name HA  ))
     5.000      5.000      0.500 peak 22332 weight  0.10000E+01 volume  0.51283E+01 ppm1      1.551 ppm2      5.141
ASSI (22372)
  ( segid "BrD " and resid 69   and name HG2%)
  (( segid "BrD " and resid 66   and name HB1 ))
     4.000      4.000      1.800 peak 22372 weight  0.10000E+01 volume  0.19974E+02 ppm1      1.428 ppm2      2.726
ASSI (22382)
  ( segid "BrD " and resid 69   and name HG2%)
  (( segid "BrD " and resid 11   and name HB2 ))
     3.100      2.400      2.400 peak 22382 weight  0.10000E+01 volume  0.94667E+02 ppm1      1.425 ppm2      2.612
ASSI (22452)
  ( segid "BrD " and resid 69   and name HG2%)
  ( segid "BrD " and resid 61   and name HD1%)
     2.400      1.400      1.400 peak 22452 weight  0.10000E+01 volume  0.42940E+01 ppm1      1.425 ppm2      1.659
ASSI (22482)
  ( segid "BrD " and resid 49   and name HG2%)
  (( segid "BrD " and resid 50   and name HG12))
     4.000      4.000      1.500 peak 22482 weight  0.10000E+01 volume  0.18478E+02 ppm1      1.568 ppm2      0.808
ASSI (22492)
  ( segid "BrD " and resid 49   and name HG2%)
  (( segid "BrD " and resid 87   and name HA  ))
     4.900      4.900      0.600 peak 22492 weight  0.10000E+01 volume  0.59811E+01 ppm1      1.569 ppm2      4.854
ASSI (22552)
  ( segid "BrD " and resid 49   and name HG1%)
  (( segid "BrD " and resid 50   and name HG12))
     4.400      4.800      0.700 peak 22552 weight  0.10000E+01 volume  0.66665E+01 ppm1      1.647 ppm2      0.835
ASSI (22592)
  (( segid "BrD " and resid 57   and name HG2 ))
  (( segid "BrD " and resid 36   and name HA  ))
     3.500      3.100      2.000 peak 22592 weight  0.10000E+01 volume  0.41488E+02 ppm1      2.016 ppm2      5.446
ASSI (22612)
  (( segid "BrD " and resid 42   and name HA  ))
  ( segid "BrD " and resid 43   and name HB% )
     4.300      4.300      1.200 peak 22612 weight  0.10000E+01 volume  0.12059E+02 ppm1      5.050 ppm2      1.710
ASSI (22632)
  (( segid "BrD " and resid 42   and name HA  ))
  (( segid "BrD " and resid 44   and name HD1 ))
     4.200      4.200      1.300 peak 22632 weight  0.10000E+01 volume  0.14713E+02 ppm1      5.051 ppm2      4.337
ASSI (22642)
  (( segid "BrD " and resid 42   and name HA  ))
  (( segid "BrD " and resid 43   and name HA  ))
     4.000      4.000      1.500 peak 22642 weight  0.10000E+01 volume  0.19305E+02 ppm1      5.051 ppm2      5.550
ASSI (22682)
  (( segid "BrD " and resid 117  and name HA  ))
  (( segid "BrD " and resid 116  and name HA  ))
     3.200      2.600      2.300 peak 22682 weight  0.10000E+01 volume  0.76840E+02 ppm1      5.148 ppm2      4.826
ASSI (22722)
  (( segid "BrD " and resid 117  and name HA  ))
  ( segid "BrD " and resid 116  and name HD1%)
     4.300      4.300      1.200 peak 22722 weight  0.10000E+01 volume  0.13070E+02 ppm1      5.149 ppm2      1.409
OR (22722)
  (( segid "BrD " and resid 117  and name HA  ))
  ( segid "BrD " and resid 116  and name HG2%)
ASSI (22732)
  (( segid "BrD " and resid 7    and name HB1 ))
  (( segid "BrD " and resid 8    and name HD2 ))
     2.400      2.000      2.000 peak 22732 weight  0.10000E+01 volume  0.18127E+03 ppm1      2.626 ppm2      4.287
ASSI (22742)
  (( segid "BrD " and resid 37   and name HA  ))
  (( segid "BrD " and resid 38   and name HA  ))
     3.900      3.800      1.600 peak 22742 weight  0.10000E+01 volume  0.31223E+02 ppm1      4.853 ppm2      4.167
ASSI (22752)
  (( segid "BrD " and resid 37   and name HA  ))
  (( segid "BrD " and resid 38   and name HB  ))
     5.500      5.500      0.000 peak 22752 weight  0.10000E+01 volume  0.13492E+00 ppm1      4.853 ppm2      1.758
ASSI (22852)
  (( segid "BrD " and resid 59   and name HB2 ))
  ( segid "BrD " and resid 56   and name HD2%)
     3.300      2.700      2.200 peak 22852 weight  0.10000E+01 volume  0.58772E+02 ppm1      2.486 ppm2      1.266
ASSI (22882)
  (( segid "BrD " and resid 8    and name HD2 ))
  (( segid "BrD " and resid 8    and name HA  ))
     3.300      2.700      2.200 peak 22882 weight  0.10000E+01 volume  0.65959E+02 ppm1      4.261 ppm2      5.021
ASSI (22892)
  (( segid "BrD " and resid 8    and name HD1 ))
  (( segid "BrD " and resid 8    and name HA  ))
     2.800      2.000      2.000 peak 22892 weight  0.10000E+01 volume  0.15205E+03 ppm1      4.407 ppm2      5.019
ASSI (22932)
  (( segid "BrD " and resid 37   and name HD1 ))
  (( segid "BrD " and resid 37   and name HA  ))
     3.000      2.200      2.200 peak 22932 weight  0.10000E+01 volume  0.11242E+03 ppm1      4.261 ppm2      4.859
ASSI (22952)
  (( segid "BrD " and resid 44   and name HD2 ))
  (( segid "BrD " and resid 42   and name HA  ))
     3.600      3.200      1.900 peak 22952 weight  0.10000E+01 volume  0.34019E+02 ppm1      4.114 ppm2      5.046
ASSI (22962)
  (( segid "BrD " and resid 91   and name HD2 ))
  (( segid "BrD " and resid 93   and name HB2 ))
     3.000      2.200      2.200 peak 22962 weight  0.10000E+01 volume  0.11249E+03 ppm1      4.409 ppm2      4.745
ASSI (22992)
  (( segid "BrD " and resid 11   and name HD1 ))
  (( segid "BrD " and resid 11   and name HB1 ))
     2.500      1.800      1.600 peak 22992 weight  0.10000E+01 volume  0.33828E+03 ppm1      4.457 ppm2      2.945
ASSI (23012)
  (( segid "BrD " and resid 8    and name HD1 ))
  (( segid "BrD " and resid 8    and name HB1 ))
     3.300      2.700      2.200 peak 23012 weight  0.10000E+01 volume  0.56548E+02 ppm1      4.409 ppm2      2.849
ASSI (23022)
  (( segid "BrD " and resid 44   and name HD1 ))
  (( segid "BrD " and resid 44   and name HG1 ))
     2.100      1.100      1.100 peak 23022 weight  0.10000E+01 volume  0.84503E+03 ppm1      4.311 ppm2      2.727
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ASSI (23062)
  (( segid "BrD " and resid 37   and name HD1 ))
  (( segid "BrD " and resid 37   and name HB2 ))
    3.200      2.600      2.300 peak 23062 weight  0.10000E+01 volume  0.68384E+02 ppm1      4.261 ppm2      2.287
ASSI (23082)
  (( segid "BrD " and resid 91   and name HD1 ))
  (( segid "BrD " and resid 91   and name HG1 ))
    2.600      1.700      1.700 peak 23082 weight  0.10000E+01 volume  0.26320E+03 ppm1      4.557 ppm2      2.784
ASSI (23092)
  (( segid "BrD " and resid 44   and name HD2 ))
  (( segid "BrD " and resid 44   and name HG1 ))
    2.300      1.300      1.300 peak 23092 weight  0.10000E+01 volume  0.51719E+03 ppm1      4.114 ppm2      2.735
ASSI (23102)
  (( segid "BrD " and resid 44   and name HD2 ))
  (( segid "BrD " and resid 44   and name HG2 ))
    2.300      1.300      1.300 peak 23102 weight  0.10000E+01 volume  0.54971E+03 ppm1      4.114 ppm2      2.654
ASSI (23112)
  (( segid "BrD " and resid 11   and name HD1 ))
  (( segid "BrD " and resid 11   and name HG1 ))
    2.600      1.700      1.700 peak 23112 weight  0.10000E+01 volume  0.26059E+03 ppm1      4.454 ppm2      2.648
ASSI (23122)
  (( segid "BrD " and resid 44   and name HD2 ))
  (( segid "BrD " and resid 44   and name HB1 ))
    2.700      1.800      1.800 peak 23122 weight  0.10000E+01 volume  0.21568E+03 ppm1      4.124 ppm2      2.973
ASSI (23202)
  (( segid "BrD " and resid 44   and name HG2 ))
  (( segid "BrD " and resid 41   and name HA  ))
    3.200      2.600      2.300 peak 23202 weight  0.10000E+01 volume  0.75568E+02 ppm1      2.635 ppm2      4.666
ASSI (23242)
  (( segid "BrD " and resid 11   and name HG1 ))
  (  segid "BrD " and resid 69   and name HG1% )
    3.200      2.600      2.300 peak 23242 weight  0.10000E+01 volume  0.73085E+02 ppm1      2.635 ppm2      1.547
ASSI (23272)
  (( segid "BrD " and resid 11   and name HG1 ))
  (  segid "BrD " and resid 14   and name HD2% )
    3.500      3.100      2.000 peak 23272 weight  0.10000E+01 volume  0.45861E+02 ppm1      2.635 ppm2      1.376
OR (23272)
  (( segid "BrD " and resid 11   and name HG1 ))
  (  segid "BrD " and resid 14   and name HD1% )
ASSI (23292)
  (( segid "BrD " and resid 91   and name HG1 ))
  (( segid "BrD " and resid 89   and name HA  ))
    4.600      4.600      0.900 peak 23292 weight  0.10000E+01 volume  0.80378E+01 ppm1      2.784 ppm2      5.646
ASSI (23372)
  (( segid "BrD " and resid 9    and name HD1 ))
  (  segid "BrD " and resid 14   and name HD1% )
    3.700      3.400      1.800 peak 23372 weight  0.10000E+01 volume  0.32255E+02 ppm1      1.768 ppm2      1.425
OR (23372)
  (( segid "BrD " and resid 9    and name HD1 ))
  (  segid "BrD " and resid 14   and name HD2% )
ASSI (23402)
  (( segid "BrD " and resid 100  and name HA  ))
  (( segid "BrD " and resid 86   and name HE1 ))
    3.500      3.100      2.000 peak 23402 weight  0.10000E+01 volume  0.44085E+03 ppm1      4.952 ppm2      3.093
ASSI (23422)
  (( segid "BrD " and resid 9    and name HB2 ))
  (( segid "BrD " and resid 8    and name HA  ))
    3.000      2.200      2.200 peak 23422 weight  0.10000E+01 volume  0.11322E+03 ppm1      3.388 ppm2      5.029
ASSI (23472)
  (( segid "BrD " and resid 6    and name HA  ))
  (( segid "BrD " and resid 6    and name HG1 ))
    1.900      0.900      0.900 peak 23472 weight  0.10000E+01 volume  0.18609E+04 ppm1      4.952 ppm2      2.214
ASSI (23572)
  (( segid "BrD " and resid 11   and name HB2 ))
  (( segid "BrD " and resid 10   and name HA  ))
    3.600      3.200      1.900 peak 23572 weight  0.10000E+01 volume  0.38586E+02 ppm1      2.585 ppm2      5.477
ASSI (23592)
  (( segid "BrD " and resid 12   and name HA  ))
  (( segid "BrD " and resid 11   and name HA  ))
    4.600      4.600      0.900 peak 23592 weight  0.10000E+01 volume  0.79375E+01 ppm1      5.297 ppm2      4.948
ASSI (23602)
  (( segid "BrD " and resid 29   and name HG1 ))
  (( segid "BrD " and resid 27   and name HA  ))
    3.900      3.800      1.600 peak 23602 weight  0.10000E+01 volume  0.21350E+02 ppm1      2.978 ppm2      5.022
ASSI (23632)
  (( segid "BrD " and resid 13   and name HB1 ))
  (( segid "BrD " and resid 113  and name HA  ))
    2.700      1.800      1.800 peak 23632 weight  0.10000E+01 volume  0.21427E+03 ppm1      2.733 ppm2      4.920
ASSI (23642)
  (( segid "BrD " and resid 13   and name HG2 ))
  (( segid "BrD " and resid 113  and name HA  ))
    3.200      2.600      2.300 peak 23642 weight  0.10000E+01 volume  0.71312E+02 ppm1      2.978 ppm2      4.920
ASSI (23652)
  (( segid "BrD " and resid 13   and name HB1 ))
  (( segid "BrD " and resid 12   and name HB2 ))
    2.900      2.100      2.100 peak 23652 weight  0.10000E+01 volume  0.14282E+03 ppm1      2.732 ppm2      3.359
ASSI (23672)
  (( segid "BrD " and resid 14   and name HA  ))
  (  segid "BrD " and resid 18   and name HD2% )
    3.300      2.700      2.200 peak 23672 weight  0.10000E+01 volume  0.64900E+02 ppm1      4.654 ppm2      0.409
ASSI (23712)
  (( segid "BrD " and resid 111  and name HA  ))
  (  segid "BrD " and resid 110  and name HG2% )
    3.400      1.400      1.400 peak 23712 weight  0.10000E+01 volume  0.44849E+03 ppm1      4.656 ppm2      1.246
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ASSI (23732)
  (( segid "BrD " and resid 14   and name HB2 ))
  (  segid "BrD " and resid 14   and name HD2% )
    3.200      1.200      1.200 peak 23732 weight  0.10000E+01 volume  0.70287E+03 ppm1      2.142 ppm2      1.402
OR (23732)
  (( segid "BrD " and resid 14   and name HB2 ))
  (  segid "BrD " and resid 14   and name HD1% )
ASSI (23762)
  (  segid "BrD " and resid 14   and name HD2% )
  (( segid "BrD " and resid 70   and name HA  ))
    3.100      2.400      2.400 peak 23762 weight  0.10000E+01 volume  0.94978E+02 ppm1      1.401 ppm2      5.359
ASSI (23802)
  (  segid "BrD " and resid 14   and name HD2% )
  (( segid "BrD " and resid 15   and name HB1 ))
    3.800      3.600      1.700 peak 23802 weight  0.10000E+01 volume  0.26555E+02 ppm1      1.401 ppm2      3.785
ASSI (23842)
  (  segid "BrD " and resid 14   and name HD2% )
  (  segid "BrD " and resid 75   and name HE% )
    2.600      1.700      1.700 peak 23842 weight  0.10000E+01 volume  0.23698E+03 ppm1      1.401 ppm2      2.619
ASSI (23882)
  (( segid "BrD " and resid 18   and name HA  ))
  (( segid "BrD " and resid 17   and name HB  ))
    3.500      3.100      2.000 peak 23882 weight  0.10000E+01 volume  0.41356E+02 ppm1      3.867 ppm2      4.867
ASSI (23922)
  (( segid "BrD " and resid 18   and name HB1 ))
  (  segid "BrD " and resid 63   and name HD2% )
    2.900      2.600      1.600 peak 23922 weight  0.10000E+01 volume  0.21833E+02 ppm1      2.144 ppm2      1.493
ASSI (23972)
  (( segid "BrD " and resid 18   and name HB2 ))
  (  segid "BrD " and resid 74   and name HE% )
    3.200      2.600      2.300 peak 23972 weight  0.10000E+01 volume  0.77951E+02 ppm1      0.911 ppm2      7.533
ASSI (23982)
  (( segid "BrD " and resid 18   and name HB2 ))
  (  segid "BrD " and resid 74   and name HD% )
    3.700      3.400      1.800 peak 23982 weight  0.10000E+01 volume  0.32246E+02 ppm1      0.911 ppm2      7.014
ASSI (24022)
  (( segid "BrD " and resid 18   and name HG  ))
  (  segid "BrD " and resid 115  and name HD1% )
    4.500      4.500      1.000 peak 24022 weight  0.10000E+01 volume  0.94731E+01 ppm1      2.290 ppm2      1.317
ASSI (24032)
  (  segid "BrD " and resid 18   and name HD2% )
  (( segid "BrD " and resid 75   and name HA  ))
    3.400      2.900      2.100 peak 24032 weight  0.10000E+01 volume  0.52852E+02 ppm1      0.415 ppm2      4.541
ASSI (24202)
  (  segid "BrD " and resid 18   and name HD1% )
  (( segid "BrD " and resid 17   and name HB  ))
    3.900      3.800      1.600 peak 24202 weight  0.10000E+01 volume  0.21965E+02 ppm1      1.056 ppm2      4.859
ASSI (24232)
  (  segid "BrD " and resid 18   and name HD1% )
  (( segid "BrD " and resid 15   and name HB1 ))
    3.700      3.400      1.800 peak 24232 weight  0.10000E+01 volume  0.32596E+02 ppm1      1.056 ppm2      3.801
ASSI (24262)
  (  segid "BrD " and resid 18   and name HD1% )
  (  segid "BrD " and resid 74   and name HD2% )
    3.500      3.100      2.000 peak 24262 weight  0.10000E+01 volume  0.41978E+02 ppm1      1.056 ppm2      0.676
ASSI (24272)
  (  segid "BrD " and resid 18   and name HD1% )
  (( segid "BrD " and resid 69   and name HA  ))
    3.400      2.900      2.100 peak 24272 weight  0.10000E+01 volume  0.49516E+02 ppm1      1.057 ppm2      4.692
ASSI (24302)
  (( segid "BrD " and resid 63   and name HA  ))
  (( segid "BrD " and resid 68   and name HB2 ))
    3.300      2.700      2.200 peak 24302 weight  0.10000E+01 volume  0.61304E+02 ppm1      5.294 ppm2      3.557
ASSI (24452)
  (( segid "BrD " and resid 63   and name HG  ))
  (( segid "BrD " and resid 68   and name HB2 ))
    3.400      2.900      2.100 peak 24452 weight  0.10000E+01 volume  0.51423E+02 ppm1      2.437 ppm2      3.516
ASSI (24462)
  (( segid "BrD " and resid 63   and name HG  ))
  (( segid "BrD " and resid 15   and name HA  ))
    2.500      2.500      2.000 peak 24462 weight  0.10000E+01 volume  0.29638E+03 ppm1      2.437 ppm2      4.645
ASSI (24482)
  (  segid "BrD " and resid 63   and name HD1% )
  (( segid "BrD " and resid 18   and name HA  ))
    3.600      3.200      1.900 peak 24482 weight  0.10000E+01 volume  0.38413E+02 ppm1      1.649 ppm2      3.878
ASSI (24512)
  (  segid "BrD " and resid 63   and name HD1% )
  (( segid "BrD " and resid 68   and name HB2 ))
    2.900      2.100      2.100 peak 24512 weight  0.10000E+01 volume  0.12236E+03 ppm1      1.649 ppm2      3.527
ASSI (24542)
  (  segid "BrD " and resid 63   and name HD1% )
  (  segid "BrD " and resid 74   and name HD% )
    3.200      2.600      2.300 peak 24542 weight  0.10000E+01 volume  0.76917E+02 ppm1      1.648 ppm2      7.006
ASSI (24682)
  (( segid "BrD " and resid 19   and name HA  ))
  (  segid "BrD " and resid 22   and name HD2% )
    3.100      2.400      2.400 peak 24682 weight  0.10000E+01 volume  0.84277E+02 ppm1      4.311 ppm2      1.588
ASSI (24702)
  (( segid "BrD " and resid 19   and name HA  ))
  (( segid "BrD " and resid 19   and name HE1 ))
    3.100      2.400      2.400 peak 24702 weight  0.10000E+01 volume  0.84024E+02 ppm1      4.310 ppm2      3.544
ASSI (24782)
  (( segid "BrD " and resid 19   and name HG1 ))
  (  segid "BrD " and resid 15   and name HE% )
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    3.300      2.700      2.200 peak 24782 weight  0.10000E+01 volume  0.57590E+02 ppm1      1.895 ppm2      7.487
ASSI {24832}
  (( segid "BrD " and resid 19    and name HD1 ))
  (  segid "BrD " and resid 15    and name HE% )
    2.400      1.400      1.400 peak 24832 weight  0.10000E+01 volume  0.37891E+03 ppm1      2.191 ppm2      7.469
ASSI {24842}
  (( segid "BrD " and resid 19    and name HD1 ))
  (  segid "BrD " and resid 63    and name HD1%)
    2.200      2.200      2.300 peak 24842 weight  0.10000E+01 volume  0.74436E+03 ppm1      2.191 ppm2      1.654
ASSI {24882}
  (( segid "BrD " and resid 23    and name HG1 ))
  (( segid "BrD " and resid 19    and name HG1 ))
    2.600      1.700      1.700 peak 24882 weight  0.10000E+01 volume  0.24553E+03 ppm1      3.124 ppm2      1.888
ASSI {24892}
  (( segid "BrD " and resid 23    and name HG2 ))
  (( segid "BrD " and resid 19    and name HG1 ))
    2.500      1.600      1.600 peak 24892 weight  0.10000E+01 volume  0.29588E+03 ppm1      3.068 ppm2      1.888
ASSI {25012}
  (( segid "BrD " and resid 21    and name HB  ))
  (  segid "BrD " and resid 106   and name HD% )
    2.400      1.400      1.400 peak 25012 weight  0.10000E+01 volume  0.42303E+03 ppm1      2.486 ppm2      7.519
ASSI {25022}
  (( segid "BrD " and resid 21    and name HG12))
  (  segid "BrD " and resid 106   and name HD% )
    4.300      4.300      1.200 peak 25022 weight  0.10000E+01 volume  0.12393E+02 ppm1      1.648 ppm2      7.511
ASSI {25072}
  (( segid "BrD " and resid 21    and name HG12))
  (  segid "BrD " and resid 17    and name HG2%)
    2.800      2.000      2.000 peak 25072 weight  0.10000E+01 volume  0.15768E+03 ppm1      1.648 ppm2      1.746
ASSI {25082}
  (( segid "BrD " and resid 21    and name HG11))
  (  segid "BrD " and resid 17    and name HG2%)
    2.200      1.200      1.200 peak 25082 weight  0.10000E+01 volume  0.65857E+03 ppm1      2.336 ppm2      1.746
ASSI {25092}
  (( segid "BrD " and resid 21    and name HG11))
  (  segid "BrD " and resid 102   and name HD2%)
    3.800      3.600      1.700 peak 25092 weight  0.10000E+01 volume  0.25380E+02 ppm1      2.336 ppm2      1.322
OR {25092}
  (( segid "BrD " and resid 21    and name HG11))
  (  segid "BrD " and resid 102   and name HD1%)
ASSI {25102}
  (( segid "BrD " and resid 21    and name HG12))
  (( segid "BrD " and resid 20    and name HB1 ))
    3.300      2.700      2.200 peak 25102 weight  0.10000E+01 volume  0.61127E+02 ppm1      1.648 ppm2      4.647
ASSI {25132}
  (( segid "BrD " and resid 62    and name HG1 ))
  (( segid "BrD " and resid 62    and name HG2 ))
    2.200      1.200      1.200 peak 25132 weight  0.10000E+01 volume  0.61439E+03 ppm1      2.336 ppm2      1.498
ASSI {25192}
  (  segid "BrD " and resid 21    and name HD1%)
  (  segid "BrD " and resid 102   and name HD2%)
    2.800      2.000      2.000 peak 25192 weight  0.10000E+01 volume  0.17249E+03 ppm1      1.205 ppm2      1.312
ASSI {25202}
  (  segid "BrD " and resid 21    and name HD1%)
  (( segid "BrD " and resid 18    and name HB2 ))
    3.400      2.900      2.100 peak 25202 weight  0.10000E+01 volume  0.54202E+02 ppm1      1.205 ppm2      0.902
ASSI {25272}
  (  segid "BrD " and resid 21    and name HG2%)
  (  segid "BrD " and resid 106   and name HE% )
    2.800      2.000      2.000 peak 25272 weight  0.10000E+01 volume  0.17880E+03 ppm1      1.599 ppm2      7.638
ASSI {25302}
  (  segid "BrD " and resid 21    and name HG2%)
  (( segid "BrD " and resid 82    and name HZ  ))
    3.500      3.100      2.000 peak 25302 weight  0.10000E+01 volume  0.42795E+02 ppm1      1.599 ppm2      6.998
ASSI {25312}
  (  segid "BrD " and resid 101   and name HG2%)
  (( segid "BrD " and resid 30    and name HA  ))
    3.500      3.100      2.000 peak 25312 weight  0.10000E+01 volume  0.43138E+02 ppm1      1.599 ppm2      5.444
ASSI {25322}
  (( segid "BrD " and resid 101   and name HA  ))
  (( segid "BrD " and resid 100   and name HA  ))
    3.400      2.900      2.100 peak 25322 weight  0.10000E+01 volume  0.52950E+02 ppm1      4.261 ppm2      4.948
ASSI {25332}
  (( segid "BrD " and resid 101   and name HA  ))
  (( segid "BrD " and resid 100   and name HB1 ))
    3.100      2.400      2.400 peak 25332 weight  0.10000E+01 volume  0.82741E+02 ppm1      4.261 ppm2      3.475
ASSI {25342}
  (( segid "BrD " and resid 101   and name HB  ))
  (( segid "BrD " and resid 30    and name HB2 ))
    3.200      2.600      2.300 peak 25342 weight  0.10000E+01 volume  0.74692E+02 ppm1      2.536 ppm2      4.525
ASSI {25352}
  (( segid "BrD " and resid 101   and name HB  ))
  (( segid "BrD " and resid 30    and name HB1 ))
    2.900      2.100      2.100 peak 25352 weight  0.10000E+01 volume  0.14018E+03 ppm1      2.536 ppm2      4.932
ASSI {25362}
  (( segid "BrD " and resid 101   and name HB  ))
  (  segid "BrD " and resid 102   and name HD1%)
    3.500      3.100      2.000 peak 25362 weight  0.10000E+01 volume  0.47210E+02 ppm1      2.536 ppm2      1.311
ASSI {25382}
  (( segid "BrD " and resid 98    and name HA  ))
  (  segid "BrD " and resid 102   and name HD1%)
    5.100      5.100      0.400 peak 25382 weight  0.10000E+01 volume  0.46968E+01 ppm1      4.804 ppm2      1.311
ASSI {25402}
  (( segid "BrD " and resid 98    and name HA  ))
  (( segid "BrD " and resid 30    and name HA  ))
    3.300      2.700      2.200 peak 25402 weight  0.10000E+01 volume  0.66772E+02 ppm1      4.804 ppm2      5.444
ASSI {25412}
  (( segid "BrD " and resid 98    and name HA  ))
  (  segid "BrD " and resid 34    and name HE% )
    3.700      3.400      1.800 peak 25412 weight  0.10000E+01 volume  0.30316E+02 ppm1      4.804 ppm2      7.779
ASSI {25422}
  (( segid "BrD " and resid 98    and name HB1 ))
  (( segid "BrD " and resid 30    and name HB1 ))
    2.900      2.100      2.100 peak 25422 weight  0.10000E+01 volume  0.12678E+03 ppm1      4.013 ppm2      4.933
ASSI {25442}
  (( segid "BrD " and resid 98    and name HB1 ))
  (( segid "BrD " and resid 30    and name HB2 ))
    3.300      2.700      2.200 peak 25442 weight  0.10000E+01 volume  0.62906E+02 ppm1      4.015 ppm2      4.533
ASSI {25452}
  (( segid "BrD " and resid 85    and name HB2 ))
  (  segid "BrD " and resid 99    and name HB% )
    2.500      1.600      1.600 peak 25452 weight  0.10000E+01 volume  0.29534E+03 ppm1      3.620 ppm2      2.206
ASSI {25462}
  (( segid "BrD " and resid 85    and name HB1 ))
  (  segid "BrD " and resid 99    and name HB% )
    2.800      2.000      2.000 peak 25462 weight  0.10000E+01 volume  0.15410E+03 ppm1      3.916 ppm2      2.206
ASSI {25502}
  (( segid "BrD " and resid 98    and name HB2 ))
  (( segid "BrD " and resid 34    and name HZ  ))
    2.900      2.100      2.100 peak 25502 weight  0.10000E+01 volume  0.12121E+03 ppm1      3.670 ppm2      7.893
ASSI {25512}
  (( segid "BrD " and resid 85    and name HB2 ))
  (  segid "BrD " and resid 34    and name HE% )
    2.400      1.400      1.400 peak 25512 weight  0.10000E+01 volume  0.45042E+03 ppm1      3.620 ppm2      7.779
ASSI {25522}
  (( segid "BrD " and resid 85    and name HB1 ))
  (  segid "BrD " and resid 34    and name HE% )
    2.500      1.600      1.600 peak 25522 weight  0.10000E+01 volume  0.32323E+03 ppm1      3.917 ppm2      7.778
ASSI {25562}
  (  segid "BrD " and resid 101   and name HD1%)
  (( segid "BrD " and resid 30    and name HB2 ))
    3.500      3.100      2.000 peak 25562 weight  0.10000E+01 volume  0.41073E+02 ppm1      1.551 ppm2      4.532
ASSI {25572}
  (  segid "BrD " and resid 101   and name HD1%)
  (( segid "BrD " and resid 30    and name HB1 ))
    3.000      2.200      2.200 peak 25572 weight  0.10000E+01 volume  0.10658E+03 ppm1      1.549 ppm2      4.932
ASSI {25582}
  (  segid "BrD " and resid 21    and name HG2%)
  (  segid "BrD " and resid 18    and name HD2%)
    3.600      3.200      1.900 peak 25582 weight  0.10000E+01 volume  0.38225E+02 ppm1      1.599 ppm2      0.408
ASSI {25642}
  (  segid "BrD " and resid 21    and name HG2%)
  (( segid "BrD " and resid 24    and name HG2 ))
    3.600      3.200      1.900 peak 25642 weight  0.10000E+01 volume  0.38422E+02 ppm1      1.599 ppm2      3.069
ASSI {25652}
  (  segid "BrD " and resid 21    and name HG2%)
  (( segid "BrD " and resid 109   and name HE2 ))
    4.000      4.000      1.500 peak 25652 weight  0.10000E+01 volume  0.20266E+02 ppm1      1.599 ppm2      3.012
ASSI {25722}
  (  segid "BrD " and resid 21    and name HG2%)
  (( segid "BrD " and resid 109   and name HB2 ))
    2.700      1.800      1.800 peak 25722 weight  0.10000E+01 volume  0.18743E+03 ppm1      1.599 ppm2      2.157
ASSI {25752}
  (  segid "BrD " and resid 101   and name HD1%)
  (( segid "BrD " and resid 102   and name HB1 ))
    3.100      2.400      2.400 peak 25752 weight  0.10000E+01 volume  0.84468E+02 ppm1      1.549 ppm2      1.970
ASSI {25812}
  (( segid "BrD " and resid 110   and name HB  ))
  (  segid "BrD " and resid 116   and name HD1%)
    2.300      1.300      1.300 peak 25812 weight  0.10000E+01 volume  0.55301E+03 ppm1      2.338 ppm2      1.410
ASSI {25822}
  (( segid "BrD " and resid 110   and name HG11))
  (  segid "BrD " and resid 78    and name HD2%)
    4.000      4.000      1.500 peak 25822 weight  0.10000E+01 volume  0.19996E+02 ppm1      1.697 ppm2      0.676
ASSI {25842}
  (  segid "BrD " and resid 110   and name HD1%)
  (( segid "BrD " and resid 75    and name HA  ))
    3.100      2.400      2.400 peak 25842 weight  0.10000E+01 volume  0.86474E+02 ppm1      1.154 ppm2      4.511
ASSI {25852}
  (  segid "BrD " and resid 110   and name HG2%)
  (( segid "BrD " and resid 114   and name HA1 ))
    4.200      4.200      1.300 peak 25852 weight  0.10000E+01 volume  0.14960E+02 ppm1      1.254 ppm2      4.569
ASSI {25952}
  (  segid "BrD " and resid 110   and name HG2%)
  (  segid "BrD " and resid 107   and name HD% )
    3.200      2.600      2.300 peak 25952 weight  0.10000E+01 volume  0.71378E+02 ppm1      1.251 ppm2      7.789
ASSI {26002}
  (  segid "BrD " and resid 110   and name HD1%)
  (  segid "BrD " and resid 106   and name HE% )
    2.500      1.600      1.600 peak 26002 weight  0.10000E+01 volume  0.29658E+03 ppm1      1.155 ppm2      7.638
ASSI {26012}
  (  segid "BrD " and resid 110   and name HD1%)
  (  segid "BrD " and resid 106   and name HD% )
    2.700      1.800      1.800 peak 26012 weight  0.10000E+01 volume  0.22034E+03 ppm1      1.155 ppm2      7.529
ASSI {26082}
  (  segid "BrD " and resid 110   and name HD1%)
  (( segid "BrD " and resid 118   and name HB1 ))
    2.300      1.300      1.300 peak 26082 weight  0.10000E+01 volume  0.81139E+03 ppm1      1.194 ppm2      2.182
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ASSI (26092)
  (  segid "BrD " and resid 110  and name HG2%)
  (( segid "BrD " and resid 111  and name HB1 ))
     3.400     2.900     2.100 peak 26092 weight  0.10000E+01 volume  0.52641E+02 ppm1      1.254 ppm2      2.493
ASSI (26122)
  (  segid "BrD " and resid 110  and name HG2%)
  (( segid "BrD " and resid 116  and name HG11))
     3.700     3.400     1.800 peak 26122 weight  0.10000E+01 volume  0.30456E+02 ppm1      1.254 ppm2      1.918
ASSI (26132)
  (  segid "BrD " and resid 110  and name HD1%)
  (( segid "BrD " and resid 116  and name HG11))
     3.300     2.700     2.200 peak 26132 weight  0.10000E+01 volume  0.58180E+02 ppm1      1.154 ppm2      1.918
ASSI (26142)
  (  segid "BrD " and resid 110  and name HD1%)
  (  segid "BrD " and resid 113  and name HB% )
     2.400     1.400     1.400 peak 26142 weight  0.10000E+01 volume  0.40630E+03 ppm1      1.154 ppm2      1.978
ASSI (26212)
  (  segid "BrD " and resid 116  and name HG2%)
  (( segid "BrD " and resid 117  and name HA  ))
     4.200     4.200     1.300 peak 26212 weight  0.10000E+01 volume  0.13762E+02 ppm1      1.401 ppm2      5.168
ASSI (26222)
  (  segid "BrD " and resid 116  and name HG2%)
  (( segid "BrD " and resid 79   and name HB2 ))
     3.200     2.600     2.300 peak 26222 weight  0.10000E+01 volume  0.79045E+02 ppm1      1.401 ppm2      2.662
ASSI (26242)
  (  segid "BrD " and resid 116  and name HG2%)
  (( segid "BrD " and resid 115  and name HB1 ))
     3.800     3.600     1.700 peak 26242 weight  0.10000E+01 volume  0.25845E+02 ppm1      1.401 ppm2      2.175
ASSI (26252)
  (  segid "BrD " and resid 116  and name HG2%)
  (( segid "BrD " and resid 116  and name HG11))
     2.700     1.800     1.800 peak 26252 weight  0.10000E+01 volume  0.22212E+03 ppm1      1.401 ppm2      1.906
ASSI (26262)
  (  segid "BrD " and resid 116  and name HG2%)
  (  segid "BrD " and resid 110  and name HD1%)
     2.400     2.400     2.100 peak 26262 weight  0.10000E+01 volume  0.45578E+03 ppm1      1.401 ppm2      1.140
ASSI (26322)
  (  segid "BrD " and resid 116  and name HD1%)
  (( segid "BrD " and resid 107  and name HA  ))
     3.200     2.600     2.300 peak 26322 weight  0.10000E+01 volume  0.76194E+02 ppm1      1.401 ppm2      4.427
ASSI (26372)
  (  segid "BrD " and resid 116  and name HD1%)
  (( segid "BrD " and resid 75   and name HG1 ))
     3.200     2.600     2.300 peak 26372 weight  0.10000E+01 volume  0.79388E+02 ppm1      1.401 ppm2      3.508
ASSI (26382)
  (  segid "BrD " and resid 116  and name HD1%)
  (( segid "BrD " and resid 79   and name HB2 ))
     3.400     2.900     2.100 peak 26382 weight  0.10000E+01 volume  0.54400E+02 ppm1      1.401 ppm2      2.662
ASSI (26402)
  (  segid "BrD " and resid 116  and name HD1%)
  (( segid "BrD " and resid 110  and name HG11))
     2.600     1.700     1.700 peak 26402 weight  0.10000E+01 volume  0.24061E+03 ppm1      1.401 ppm2      1.718
ASSI (26412)
  (  segid "BrD " and resid 116  and name HD1%)
  (( segid "BrD " and resid 110  and name HG12))
     2.100     1.100     1.100 peak 26412 weight  0.10000E+01 volume  0.93798E+03 ppm1      1.401 ppm2      1.637
ASSI (26432)
  (  segid "BrD " and resid 116  and name HD1%)
  (( segid "BrD " and resid 78   and name HB2 ))
     2.400     2.400     2.100 peak 26432 weight  0.10000E+01 volume  0.39159E+03 ppm1      1.399 ppm2      1.078
ASSI (26472)
  (  segid "BrD " and resid 116  and name HD1%)
  (  segid "BrD " and resid 78   and name HD2%)
     4.900     4.900     0.600 peak 26472 weight  0.10000E+01 volume  0.55118E+01 ppm1      1.399 ppm2      0.680
ASSI (26482)
  (  segid "BrD " and resid 116  and name HD1%)
  (  segid "BrD " and resid 110  and name HG2%)
     2.000     1.000     1.000 peak 26482 weight  0.10000E+01 volume  0.13707E+04 ppm1      1.399 ppm2      1.237
ASSI (26502)
  (  segid "BrD " and resid 63   and name HD2%)
  (( segid "BrD " and resid 60   and name HA  ))
     2.300     1.300     1.300 peak 26502 weight  0.10000E+01 volume  0.60749E+03 ppm1      1.501 ppm2      4.818
ASSI (26522)
  (( segid "BrD " and resid 116  and name HB  ))
  (( segid "BrD " and resid 115  and name HB1 ))
     4.400     4.400     1.100 peak 26522 weight  0.10000E+01 volume  0.11059E+02 ppm1      2.432 ppm2      2.200
ASSI (26532)
  (( segid "BrD " and resid 116  and name HB  ))
  (  segid "BrD " and resid 110  and name HG2%)
     3.600     3.200     1.900 peak 26532 weight  0.10000E+01 volume  0.35446E+02 ppm1      2.409 ppm2      1.263
ASSI (26542)
  (( segid "BrD " and resid 116  and name HB  ))
  (  segid "BrD " and resid 110  and name HD1%)
     3.300     2.700     2.300 peak 26542 weight  0.10000E+01 volume  0.65125E+02 ppm1      2.409 ppm2      1.149
ASSI (26682)
  (( segid "BrD " and resid 103  and name HG2 ))
  (( segid "BrD " and resid 104  and name HA  ))
     3.300     2.700     2.200 peak 26682 weight  0.10000E+01 volume  0.56609E+02 ppm1      2.519 ppm2      4.679
ASSI (26692)
  (( segid "BrD " and resid 94   and name HG1 ))
  (( segid "BrD " and resid 93   and name HB1 ))
     5.400     5.400     0.100 peak 26692 weight  0.10000E+01 volume  0.32972E+01 ppm1      3.127 ppm2      5.038
OR (26692)
  (( segid "BrD " and resid 94   and name HG1 ))
  (( segid "BrD " and resid 93   and name HA  ))
ASSI (26702)
  (( segid "BrD " and resid 94   and name HG1 ))
  (( segid "BrD " and resid 95   and name HA  ))
     3.700     3.400     1.800 peak 26702 weight  0.10000E+01 volume  0.33522E+02 ppm1      3.132 ppm2      4.448
ASSI (26752)
  (( segid "BrD " and resid 96   and name HG1 ))
  (( segid "BrD " and resid 97   and name HD1 ))
     2.600     1.700     1.700 peak 26752 weight  0.10000E+01 volume  0.26306E+03 ppm1      3.127 ppm2      2.401
ASSI (26872)
  (( segid "BrD " and resid 86   and name HD1 ))
  (( segid "BrD " and resid 87   and name HG1 ))
     2.700     1.800     1.800 peak 26872 weight  0.10000E+01 volume  0.22393E+03 ppm1      1.892 ppm2      3.028
ASSI (26902)
  (( segid "BrD " and resid 36   and name HG1 ))
  (( segid "BrD " and resid 57   and name HG2 ))
     3.500     3.100     2.000 peak 26902 weight  0.10000E+01 volume  0.44296E+02 ppm1      2.781 ppm2      2.003
ASSI (26922)
  (( segid "BrD " and resid 37   and name HB1 ))
  (( segid "BrD " and resid 56   and name HA  ))
     4.000     4.000     1.500 peak 26922 weight  0.10000E+01 volume  0.19758E+02 ppm1      2.930 ppm2      5.662
ASSI (26952)
  (( segid "BrD " and resid 37   and name HG1 ))
  (( segid "BrD " and resid 36   and name HA  ))
     5.300     5.300     0.200 peak 26952 weight  0.10000E+01 volume  0.36066E+01 ppm1      2.733 ppm2      5.444
ASSI (26962)
  (( segid "BrD " and resid 112  and name HG2 ))
  (( segid "BrD " and resid 111  and name HG2 ))
     3.400     2.900     2.100 peak 26962 weight  0.10000E+01 volume  0.56268E+02 ppm1      2.815 ppm2      1.898
ASSI (26972)
  (( segid "BrD " and resid 61   and name HB2 ))
  (  segid "BrD " and resid 58   and name HG2%)
     3.000     2.200     2.300 peak 26972 weight  0.10000E+01 volume  0.11517E+03 ppm1      2.684 ppm2      1.644
ASSI (27022)
  (( segid "BrD " and resid 89   and name HA  ))
  (( segid "BrD " and resid 93   and name HB2 ))
     3.700     3.400     1.800 peak 27022 weight  0.10000E+01 volume  0.31951E+02 ppm1      5.642 ppm2      4.745
ASSI (27032)
  (( segid "BrD " and resid 89   and name HB1 ))
  (( segid "BrD " and resid 96   and name HB2 ))
     3.300     2.700     2.200 peak 27032 weight  0.10000E+01 volume  0.59751E+02 ppm1      3.669 ppm2      3.117
ASSI (27082)
  (( segid "BrD " and resid 100  and name HB2 ))
  (  segid "BrD " and resid 101  and name HD1%)
     4.000     4.000     1.500 peak 27082 weight  0.10000E+01 volume  0.18249E+02 ppm1      3.421 ppm2      1.572
OR (27082)
  (( segid "BrD " and resid 100  and name HB2 ))
  (  segid "BrD " and resid 101  and name HG2%)
ASSI (27092)
  (( segid "BrD " and resid 100  and name HB2 ))
  (( segid "BrD " and resid 101  and name HA  ))
     4.000     4.000     1.500 peak 27092 weight  0.10000E+01 volume  0.18330E+02 ppm1      3.423 ppm2      4.265
ASSI (27102)
  (( segid "BrD " and resid 100  and name HB2 ))
  (( segid "BrD " and resid 101  and name HG11))
     2.700     1.800     1.800 peak 27102 weight  0.10000E+01 volume  0.20958E+03 ppm1      3.423 ppm2      2.458
ASSI (27112)
  (( segid "BrD " and resid 100  and name HB2 ))
  (  segid "BrD " and resid 99   and name HB% )
     3.400     2.900     2.100 peak 27112 weight  0.10000E+01 volume  0.49005E+02 ppm1      3.423 ppm2      2.206
ASSI (27142)
  (( segid "BrD " and resid 80   and name HD1 ))
  (( segid "BrD " and resid 77   and name HA  ))
     3.100     2.400     2.400 peak 27142 weight  0.10000E+01 volume  0.85246E+02 ppm1      3.962 ppm2      4.963
ASSI (27172)
  (( segid "BrD " and resid 80   and name HD2 ))
  (( segid "BrD " and resid 84   and name HB2 ))
     4.100     4.100     1.400 peak 27172 weight  0.10000E+01 volume  0.16038E+02 ppm1      3.913 ppm2      3.276
ASSI (27192)
  (( segid "BrD " and resid 80   and name HD2 ))
  (( segid "BrD " and resid 83   and name HB  ))
     3.400     2.900     2.100 peak 27192 weight  0.10000E+01 volume  0.47687E+02 ppm1      3.912 ppm2      4.808
ASSI (27202)
  (( segid "BrD " and resid 80   and name HD2 ))
  (( segid "BrD " and resid 52   and name HA  ))
     3.900     3.800     1.600 peak 27202 weight  0.10000E+01 volume  0.23078E+02 ppm1      3.902 ppm2      8.983
ASSI (27322)
  (( segid "BrD " and resid 56   and name HG  ))
  (  segid "BrD " and resid 81   and name HG1%)
     3.400     2.900     2.100 peak 27322 weight  0.10000E+01 volume  0.49600E+02 ppm1      2.339 ppm2      1.079
ASSI (27342)
  (( segid "BrD " and resid 55   and name HB1 ))
  (( segid "BrD " and resid 34   and name HA  ))
     3.300     2.700     2.200 peak 27342 weight  0.10000E+01 volume  0.66937E+02 ppm1      2.979 ppm2      5.539
ASSI (27362)
  (( segid "BrD " and resid 55   and name HB1 ))
  (  segid "BrD " and resid 81   and name HG1%)
     3.900     3.800     1.600 peak 27362 weight  0.10000E+01 volume  0.24126E+02 ppm1      2.979 ppm2      1.075
ASSI (27372)
  (( segid "BrD " and resid 38   and name HA  ))
  (( segid "BrD " and resid 39   and name HA  ))
     3.300     3.100     2.000 peak 27372 weight  0.10000E+01 volume  0.46123E+02 ppm1      4.163 ppm2      4.972
ASSI (27382)
  (( segid "BrD " and resid 55   and name HB1 ))
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   (( segid "BrD " and resid 36   and name HA  ))
      3.400      2.900      2.100 peak 27392 weight  0.10000E+01 volume  0.54954E+02 ppm1      2.979 ppm2      5.442
ASSI {27442}
   (  segid "BrD " and resid 69   and name HG1%)
   (  segid "BrD " and resid 18   and name HD1%)
      2.400      2.400      2.100 peak 27442 weight  0.10000E+01 volume  0.37353E+03 ppm1      1.547 ppm2      1.091
ASSI {27452}
   (  segid "BrD " and resid 22   and name HD2%)
   (  segid "BrD " and resid 25   and name HG1%)
      2.500      1.600      1.600 peak 27452 weight  0.10000E+01 volume  0.30318E+03 ppm1      1.599 ppm2      1.788
ASSI {27472}
   (  segid "BrD " and resid 22   and name HD2%)
   (( segid "BrD " and resid 25   and name HB  ))
      3.400      2.900      2.100 peak 27472 weight  0.10000E+01 volume  0.54052E+02 ppm1      1.599 ppm2      3.003
ASSI {27492}
   (  segid "BrD " and resid 22   and name HD2%)
   (( segid "BrD " and resid 60   and name HA  ))
      2.300      1.300      1.100 peak 27492 weight  0.10000E+01 volume  0.56630E+03 ppm1      1.599 ppm2      4.809
ASSI {27552}
   (  segid "BrD " and resid 22   and name HD2%)
   (  segid "BrD " and resid 74   and name HE% )
      2.300      2.300      2.200 peak 27552 weight  0.10000E+01 volume  0.54070E+03 ppm1      1.599 ppm2      7.529
ASSI {27572}
   (  segid "BrD " and resid 22   and name HD1%)
   (( segid "BrD " and resid 60   and name HB1 ))
      3.200      2.600      2.300 peak 27572 weight  0.10000E+01 volume  0.80681E+02 ppm1      1.645 ppm2      4.990
ASSI {27582}
   (  segid "BrD " and resid 22   and name HD1%)
   (  segid "BrD " and resid 74   and name HE% )
      3.200      1.200      1.200 peak 27582 weight  0.10000E+01 volume  0.62438E+03 ppm1      1.646 ppm2      7.529
ASSI {27632}
   (  segid "BrD " and resid 73   and name HD1%)
   (( segid "BrD " and resid 68   and name HA  ))
      2.500      1.600      1.600 peak 27632 weight  0.10000E+01 volume  0.31070E+03 ppm1      1.549 ppm2      5.143
ASSI {27662}
   (  segid "BrD " and resid 73   and name HD1%)
   (( segid "BrD " and resid 70   and name HB2 ))
      3.100      2.400      2.400 peak 27662 weight  0.10000E+01 volume  0.86052E+02 ppm1      1.549 ppm2      4.362
ASSI {27692}
   (  segid "BrD " and resid 73   and name HD2%)
   (  segid "BrD " and resid 76   and name HB% )
      2.600      2.000      2.000 peak 27692 weight  0.10000E+01 volume  0.17686E+03 ppm1      1.500 ppm2      2.106
ASSI {27712}
   (( segid "BrD " and resid 35   and name HA  ))
   (( segid "BrD " and resid 56   and name HB2 ))
      2.100      1.100      1.100 peak 27712 weight  0.10000E+01 volume  0.10158E+04 ppm1      4.900 ppm2      2.004
ASSI {27722}
   (( segid "BrD " and resid 48   and name HA  ))
   (  segid "BrD " and resid 49   and name HG1%)
      3.000      2.200      2.200 peak 27722 weight  0.10000E+01 volume  0.11137E+03 ppm1      4.803 ppm2      1.652
ASSI {27772}
   (( segid "BrD " and resid 73   and name HB2 ))
   (( segid "BrD " and resid 70   and name HB2 ))
      3.400      2.900      2.100 peak 27772 weight  0.10000E+01 volume  0.55069E+02 ppm1      2.487 ppm2      4.377
ASSI {27822}
   (( segid "BrD " and resid 78   and name HA  ))
   (( segid "BrD " and resid 77   and name HB1 ))
      3.800      3.600      1.700 peak 27822 weight  0.10000E+01 volume  0.26285E+02 ppm1      3.967 ppm2      3.312
ASSI {27842}
   (( segid "BrD " and resid 78   and name HB2 ))
   (( segid "BrD " and resid 116  and name HG11))
      3.700      3.400      1.800 peak 27842 weight  0.10000E+01 volume  0.31985E+02 ppm1      1.056 ppm2      1.954
ASSI {27872}
   (( segid "BrD " and resid 76   and name HB2 ))
   (( segid "BrD " and resid 79   and name HA  ))
      4.100      4.100      1.400 peak 27872 weight  0.10000E+01 volume  0.17221E+02 ppm1      1.056 ppm2      4.411
ASSI {27882}
   (( segid "BrD " and resid 78   and name HG  ))
   (( segid "BrD " and resid 75   and name HA  ))
      5.500      5.500      0.000 peak 27882 weight  0.10000E+01 volume  0.22274E+01 ppm1      1.254 ppm2      4.509
ASSI {27892}
   (( segid "BrD " and resid 76   and name HG  ))
   (( segid "BrD " and resid 82   and name HZ  ))
      2.500      2.500      2.000 peak 27892 weight  0.10000E+01 volume  0.10077E+03 ppm1      1.254 ppm2      7.047
OR {27892}
   (( segid "BrD " and resid 78   and name HG  ))
   (  segid "BrD " and resid 82   and name HE% )
ASSI {27912}
   (( segid "BrD " and resid 78   and name HB2 ))
   (  segid "BrD " and resid 106  and name HD% )
      3.600      3.200      1.900 peak 27912 weight  0.10000E+01 volume  0.34865E+02 ppm1      1.056 ppm2      7.532
ASSI {27942}
   (  segid "BrD " and resid 78   and name HD1%)
   (  segid "BrD " and resid 106  and name HE% )
      2.600      1.700      1.700 peak 27942 weight  0.10000E+01 volume  0.24618E+03 ppm1      0.760 ppm2      7.635
ASSI {27982}
   (  segid "BrD " and resid 78   and name HD2%)
   (  segid "BrD " and resid 106  and name HD% )
      3.200      1.200      1.200 peak 27982 weight  0.10000E+01 volume  0.76393E+03 ppm1      0.662 ppm2      7.528
ASSI {27992}
   (  segid "BrD " and resid 78   and name HD2%)
   (( segid "BrD " and resid 82   and name HZ  ))
      3.100      1.100      1.100 peak 27992 weight  0.10000E+01 volume  0.83417E+03 ppm1      0.662 ppm2      7.031
OR {27992}
   (  segid "BrD " and resid 78   and name HD2%)
   (  segid "BrD " and resid 82   and name HE% )
ASSI {28012}
   (  segid "BrD " and resid 78   and name HD2%)
   (  segid "BrD " and resid 106  and name HE% )
      2.900      2.100      2.100 peak 28012 weight  0.10000E+01 volume  0.14234E+03 ppm1      0.662 ppm2      7.637
ASSI {28032}
   (  segid "BrD " and resid 78   and name HD1%)
   (( segid "BrD " and resid 22   and name HA  ))
      3.500      3.100      2.000 peak 28032 weight  0.10000E+01 volume  0.43609E+02 ppm1      0.761 ppm2      4.727
ASSI {28062}
   (  segid "BrD " and resid 78   and name HD1%)
   (( segid "BrD " and resid 75   and name HA  ))
      3.500      3.100      2.000 peak 28062 weight  0.10000E+01 volume  0.46405E+02 ppm1      0.761 ppm2      4.525
ASSI {28102}
   (  segid "BrD " and resid 78   and name HD1%)
   (( segid "BrD " and resid 106  and name HB1 ))
      4.700      4.700      0.800 peak 28102 weight  0.10000E+01 volume  0.77501E+01 ppm1      0.761 ppm2      3.918
ASSI {28122}
   (  segid "BrD " and resid 78   and name HD2%)
   (( segid "BrD " and resid 106  and name HB2 ))
      2.900      2.100      2.100 peak 28122 weight  0.10000E+01 volume  0.14435E+03 ppm1      0.662 ppm2      3.703
ASSI {28132}
   (  segid "BrD " and resid 78   and name HD2%)
   (( segid "BrD " and resid 106  and name HB1 ))
      2.900      2.100      2.100 peak 28132 weight  0.10000E+01 volume  0.12376E+03 ppm1      0.662 ppm2      3.919
ASSI {28192}
   (  segid "BrD " and resid 78   and name HD1%)
   (( segid "BrD " and resid 81   and name HB  ))
      2.700      1.800      1.800 peak 28192 weight  0.10000E+01 volume  0.18524E+03 ppm1      0.760 ppm2      2.043
ASSI {28202}
   (  segid "BrD " and resid 78   and name HD1%)
   (  segid "BrD " and resid 22   and name HD2%)
      2.500      1.600      1.600 peak 28202 weight  0.10000E+01 volume  0.29008E+03 ppm1      0.761 ppm2      1.590
ASSI {28212}
   (  segid "BrD " and resid 78   and name HD1%)
   (  segid "BrD " and resid 18   and name HD2%)
      3.300      2.700      2.200 peak 28232 weight  0.10000E+01 volume  0.64808E+02 ppm1      0.760 ppm2      0.424
ASSI {28262}
   (  segid "BrD " and resid 56   and name HD2%)
   (  segid "BrD " and resid 74   and name HE% )
      4.100      4.100      1.400 peak 28262 weight  0.10000E+01 volume  0.17777E+02 ppm1      1.254 ppm2      7.534
ASSI {28272}
   (  segid "BrD " and resid 56   and name HD2%)
   (  segid "BrD " and resid 82   and name HE% )
      3.400      2.900      2.100 peak 28272 weight  0.10000E+01 volume  0.54803E+02 ppm1      1.253 ppm2      7.041
OR {28272}
   (  segid "BrD " and resid 56   and name HD2%)
   (( segid "BrD " and resid 82   and name HZ  ))
ASSI {28292}
   (  segid "BrD " and resid 56   and name HD2%)
   (( segid "BrD " and resid 55   and name HA  ))
      3.500      3.100      2.000 peak 28292 weight  0.10000E+01 volume  0.41030E+02 ppm1      1.254 ppm2      5.371
ASSI {28322}
   (  segid "BrD " and resid 56   and name HD2%)
   (( segid "BrD " and resid 26   and name HA  ))
      3.100      2.400      2.400 peak 28322 weight  0.10000E+01 volume  0.83493E+02 ppm1      1.254 ppm2      4.509
ASSI {28342}
   (  segid "BrD " and resid 56   and name HD2%)
   (( segid "BrD " and resid 22   and name HA  ))
      3.000      2.200      2.200 peak 28342 weight  0.10000E+01 volume  0.99805E+02 ppm1      1.251 ppm2      4.733
ASSI {28352}
   (  segid "BrD " and resid 56   and name HD2%)
   (( segid "BrD " and resid 78   and name HA  ))
      3.800      3.600      1.700 peak 28352 weight  0.10000E+01 volume  0.27666E+02 ppm1      1.254 ppm2      3.996
ASSI {28372}
   (  segid "BrD " and resid 56   and name HD2%)
   (( segid "BrD " and resid 25   and name HB  ))
      3.500      3.100      2.000 peak 28372 weight  0.10000E+01 volume  0.41722E+02 ppm1      1.254 ppm2      3.003
ASSI {28402}
   (( segid "BrD " and resid 56   and name HB1 ))
   (( segid "BrD " and resid 35   and name HG1 ))
      3.800      3.600      1.700 peak 28402 weight  0.10000E+01 volume  0.28628E+02 ppm1      2.684 ppm2      3.451
ASSI {28412}
   (( segid "BrD " and resid 56   and name HB2 ))
   (( segid "BrD " and resid 35   and name HG1 ))
      4.000      4.000      1.500 peak 28412 weight  0.10000E+01 volume  0.20241E+02 ppm1      1.993 ppm2      3.443
ASSI {28442}
   (( segid "BrD " and resid 102  and name HB1 ))
   (  segid "BrD " and resid 82   and name HE% )
      2.900      2.100      2.100 peak 28442 weight  0.10000E+01 volume  0.13708E+03 ppm1      1.993 ppm2      7.064
ASSI {28472}
   (( segid "BrD " and resid 102  and name HB2 ))
   (  segid "BrD " and resid 34   and name HE% )
      3.200      2.600      2.300 peak 28472 weight  0.10000E+01 volume  0.70904E+02 ppm1      1.842 ppm2      7.778
ASSI {28502}
   (( segid "BrD " and resid 102  and name HB2 ))
   (  segid "BrD " and resid 81   and name HG2%)
      3.600      3.200      1.900 peak 28502 weight  0.10000E+01 volume  0.34445E+02 ppm1      1.842 ppm2      0.766
ASSI {28532}
   (( segid "BrD " and resid 102  and name HG  ))
   (  segid "BrD " and resid 82   and name HE% )
      2.500      1.600      1.600 peak 28532 weight  0.10000E+01 volume  0.29286E+03 ppm1      2.141 ppm2      7.041
ASSI {28562}
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   ( segid "BrD " and resid 102  and name HD2%)
   ( segid "BrD " and resid 82   and name HD% )
     3.600     3.200     1.900 peak 28562 weight  0.10000E+01 volume  0.38923E+02 ppm1     1.303 ppm2     7.245
ASSI (28582)
   ( segid "BrD " and resid 102  and name HD2%)
   ( segid "BrD " and resid 106  and name HD% )
     3.100     2.400     2.400 peak 28582 weight  0.10000E+01 volume  0.86642E+02 ppm1     1.303 ppm2     7.534
ASSI (28622)
   ( segid "BrD " and resid 102  and name HD2%)
   (( segid "BrD " and resid 28   and name HD2 ))
     3.100     2.400     2.400 peak 28622 weight  0.10000E+01 volume  0.83600E+02 ppm1     1.303 ppm2     5.553
ASSI (28632)
   ( segid "BrD " and resid 102  and name HD2%)
   (( segid "BrD " and resid 106  and name HA  ))
     2.800     2.000     3.000 peak 28632 weight  0.10000E+01 volume  0.15974E+03 ppm1     1.303 ppm2     4.525
ASSI (28642)
   ( segid "BrD " and resid 102  and name HD2%)
   (( segid "BrD " and resid 21   and name HA  ))
     3.500     3.100     2.000 peak 28642 weight  0.10000E+01 volume  0.44750E+02 ppm1     1.303 ppm2     4.354
ASSI (28662)
   ( segid "BrD " and resid 102  and name HD1%)
   (( segid "BrD " and resid 28   and name HD2 ))
     3.200     2.600     2.300 peak 28662 weight  0.10000E+01 volume  0.73306E+02 ppm1     1.303 ppm2     5.574
ASSI (28702)
   ( segid "BrD " and resid 102  and name HD2%)
   (( segid "BrD " and resid 106  and name HB1 ))
     3.600     3.200     1.900 peak 28702 weight  0.10000E+01 volume  0.36289E+02 ppm1     1.303 ppm2     3.882
ASSI (28722)
   ( segid "BrD " and resid 102  and name HD2%)
   (( segid "BrD " and resid 21   and name HB  ))
     3.200     2.600     2.300 peak 28722 weight  0.10000E+01 volume  0.68526E+02 ppm1     1.305 ppm2     2.473
ASSI (28752)
   ( segid "BrD " and resid 102  and name HD2%)
   ( segid "BrD " and resid 76   and name HD2%)
     3.400     2.900     2.100 peak 28752 weight  0.10000E+01 volume  0.55554E+02 ppm1     1.303 ppm2     0.676
ASSI (28782)
   ( segid "BrD " and resid 115  and name HD1%)
   ( segid "BrD " and resid 17   and name HG2%)
     2.200     1.200     1.200 peak 28782 weight  0.10000E+01 volume  0.67664E+03 ppm1     1.352 ppm2     1.750
ASSI (28792)
   (( segid "BrD " and resid 66   and name HG2 ))
   (( segid "BrD " and resid 65   and name HA  ))
     3.000     2.200     2.200 peak 28792 weight  0.10000E+01 volume  0.10599E+03 ppm1     2.141 ppm2     5.395
ASSI (28812)
   (( segid "BrD " and resid 115  and name HB1 ))
   (( segid "BrD " and resid 110  and name HA  ))
     2.400     1.400     1.400 peak 28812 weight  0.10000E+01 volume  0.45932E+03 ppm1     2.190 ppm2     4.419
ASSI (28822)
   (( segid "BrD " and resid 115  and name HG  ))
   (( segid "BrD " and resid 110  and name HA  ))
     2.800     2.000     2.000 peak 28822 weight  0.10000E+01 volume  0.18123E+03 ppm1     2.139 ppm2     4.426
ASSI (28842)
   (( segid "BrD " and resid 115  and name HG  ))
   ( segid "BrD " and resid 110  and name HD1%)
     3.400     2.900     2.100 peak 28842 weight  0.10000E+01 volume  0.47604E+02 ppm1     2.139 ppm2     1.140
ASSI (28852)
   (( segid "BrD " and resid 115  and name HB1 ))
   ( segid "BrD " and resid 113  and name HB% )
     3.600     3.200     1.900 peak 28852 weight  0.10000E+01 volume  0.39467E+02 ppm1     2.190 ppm2     1.978
ASSI (28872)
   (( segid "BrD " and resid 115  and name HB1 ))
   (( segid "BrD " and resid 110  and name HG12))
     2.600     2.600     1.900 peak 28872 weight  0.10000E+01 volume  0.26332E+03 ppm1     2.190 ppm2     1.661
ASSI (28882)
   (( segid "BrD " and resid 115  and name HB1 ))
   ( segid "BrD " and resid 116  and name HD1%)
     3.200     1.200     1.200 peak 28882 weight  0.10000E+01 volume  0.69706E+03 ppm1     2.188 ppm2     1.424
OR (28882)
   (( segid "BrD " and resid 115  and name HB1 ))
   ( segid "BrD " and resid 116  and name HG2%)
ASSI (28892)
   (( segid "BrD " and resid 115  and name HB1 ))
   (( segid "BrD " and resid 116  and name HG12))
     4.000     4.000     1.500 peak 28892 weight  0.10000E+01 volume  0.19745E+02 ppm1     2.188 ppm2     1.583
ASSI (28912)
   (( segid "BrD " and resid 115  and name HA  ))
   ( segid "BrD " and resid 110  and name HG2%)
     3.400     2.900     2.100 peak 28912 weight  0.10000E+01 volume  0.51456E+02 ppm1     4.807 ppm2     1.263
ASSI (28932)
   ( segid "BrD " and resid 56   and name HD1%)
   (( segid "BrD " and resid 35   and name HG1 ))
     3.600     3.200     1.900 peak 28932 weight  0.10000E+01 volume  0.33849E+02 ppm1     1.549 ppm2     3.451
ASSI (28942)
   ( segid "BrD " and resid 56   and name HD1%)
   (( segid "BrD " and resid 35   and name HA  ))
     2.800     2.000     2.000 peak 28942 weight  0.10000E+01 volume  0.16319E+03 ppm1     1.548 ppm2     4.900
ASSI (29012)
   ( segid "BrD " and resid 59   and name HE% )
   (( segid "BrD " and resid 81   and name HB  ))
     2.500     2.500     2.000 peak 29012 weight  0.10000E+01 volume  0.32346E+03 ppm1     1.848 ppm2     2.018
ASSI (29042)
   ( segid "BrD " and resid 59   and name HE% )
   (( segid "BrD " and resid 54   and name HB2 ))
     1.800     1.800     2.700 peak 29042 weight  0.10000E+01 volume  0.22344E+04 ppm1     1.848 ppm2     1.944
ASSI (29052)
   ( segid "BrD " and resid 59   and name HE% )
   (( segid "BrD " and resid 74   and name HB2 ))
     3.900     3.600     1.600 peak 29052 weight  0.10000E+01 volume  0.23714E+02 ppm1     1.848 ppm2     3.002
ASSI (29132)
   ( segid "BrD " and resid 59   and name HE% )
   (( segid "BrD " and resid 77   and name HA  ))
     3.600     3.200     1.900 peak 29132 weight  0.10000E+01 volume  0.36305E+02 ppm1     1.847 ppm2     4.966
ASSI (29142)
   ( segid "BrD " and resid 59   and name HE% )
   (( segid "BrD " and resid 75   and name HA  ))
     4.500     4.500     1.000 peak 29142 weight  0.10000E+01 volume  0.98620E+01 ppm1     1.847 ppm2     4.516
ASSI (29172)
   ( segid "BrD " and resid 54   and name HE% )
   (( segid "BrD " and resid 58   and name HA  ))
     3.500     3.100     2.000 peak 29172 weight  0.10000E+01 volume  0.40557E+02 ppm1     2.536 ppm2     4.468
ASSI (29222)
   ( segid "BrD " and resid 54   and name HE% )
   (( segid "BrD " and resid 57   and name HB2 ))
     2.800     2.000     2.000 peak 29222 weight  0.10000E+01 volume  0.17311E+03 ppm1     2.536 ppm2     2.881
ASSI (29232)
   ( segid "BrD " and resid 54   and name HE% )
   (( segid "BrD " and resid 59   and name HG2 ))
     2.900     2.100     2.100 peak 29232 weight  0.10000E+01 volume  0.12717E+03 ppm1     2.535 ppm2     3.199
OR (29232)
   ( segid "BrD " and resid 54   and name HE% )
   (( segid "BrD " and resid 59   and name HG1 ))
ASSI (29292)
   (( segid "BrD " and resid 54   and name HB2 ))
   ( segid "BrD " and resid 81   and name HG1%)
     3.200     2.600     2.300 peak 29292 weight  0.10000E+01 volume  0.80321E+02 ppm1     1.947 ppm2     1.083
ASSI (29302)
   ( segid "BrD " and resid 54   and name HE% )
   ( segid "BrD " and resid 59   and name HE% )
     3.000     2.200     2.200 peak 29302 weight  0.10000E+01 volume  0.10558E+03 ppm1     2.535 ppm2     1.863
ASSI (29382)
   (( segid "BrD " and resid 33   and name HA  ))
   (( segid "BrD " and resid 32   and name HZ3 ))
     3.200     2.600     2.300 peak 29382 weight  0.10000E+01 volume  0.67859E+02 ppm1     4.361 ppm2     7.811
ASSI (29472)
   (( segid "BrD " and resid 91   and name HG1 ))
   (( segid "BrD " and resid 93   and name HB1 ))
     2.700     3.400     1.800 peak 29472 weight  0.10000E+01 volume  0.32210E+02 ppm1     2.779 ppm2     5.018
OR (29472)
   (( segid "BrD " and resid 91   and name HG1 ))
   (( segid "BrD " and resid 93   and name HA  ))
ASSI (29602)
   (( segid "BrD " and resid 70   and name HA  ))
   (( segid "BrD " and resid 73   and name HB2 ))
     3.600     3.200     1.900 peak 29602 weight  0.10000E+01 volume  0.37115E+02 ppm1     5.346 ppm2     2.483
ASSI (29622)
   (( segid "BrD " and resid 70   and name HB2 ))
   (( segid "BrD " and resid 9    and name HB1 ))
     3.100     2.400     2.400 peak 29622 weight  0.10000E+01 volume  0.85748E+02 ppm1     4.360 ppm2     2.443
ASSI (29632)
   (( segid "BrD " and resid 70   and name HB1 ))
   (( segid "BrD " and resid 9    and name HB1 ))
     3.600     3.200     1.900 peak 29632 weight  0.10000E+01 volume  0.38576E+02 ppm1     4.755 ppm2     2.442
ASSI (29642)
   (( segid "BrD " and resid 93   and name HB2 ))
   (( segid "BrD " and resid 91   and name HD1 ))
     2.300     1.300     1.300 peak 29642 weight  0.10000E+01 volume  0.51818E+03 ppm1     4.755 ppm2     4.550
ASSI (29652)
   (( segid "BrD " and resid 93   and name HB1 ))
   (( segid "BrD " and resid 91   and name HD1 ))
     2.900     2.100     2.100 peak 29652 weight  0.10000E+01 volume  0.14178E+03 ppm1     5.000 ppm2     4.550
ASSI (29662)
   (( segid "BrD " and resid 93   and name HB1 ))
   (( segid "BrD " and resid 94   and name HB1 ))
     3.100     2.400     2.400 peak 29662 weight  0.10000E+01 volume  0.83013E+02 ppm1     5.000 ppm2     3.731
ASSI (29672)
   (( segid "BrD " and resid 93   and name HA  ))
   (( segid "BrD " and resid 91   and name HG1 ))
     3.100     2.400     2.400 peak 29672 weight  0.10000E+01 volume  0.87723E+02 ppm1     5.003 ppm2     2.798
ASSI (29692)
   (( segid "BrD " and resid 108  and name HA  ))
   (( segid "BrD " and resid 111  and name HG2 ))
     4.300     4.300     1.200 peak 29692 weight  0.10000E+01 volume  0.13111E+02 ppm1     4.804 ppm2     1.905
ASSI (29752)
   (( segid "BrD " and resid 30   and name HA  ))
   ( segid "BrD " and resid 102  and name HD1%)
     4.200     4.200     1.300 peak 29752 weight  0.10000E+01 volume  0.14252E+02 ppm1     5.445 ppm2     1.327
ASSI (29772)
   (( segid "BrD " and resid 30   and name HB2 ))
   (( segid "BrD " and resid 28   and name HE1 ))
     3.300     2.700     3.200 peak 29772 weight  0.10000E+01 volume  0.60630E+02 ppm1     4.808 ppm2     8.090
ASSI (29782)
   (( segid "BrD " and resid 30   and name HB2 ))
   ( segid "BrD " and resid 101  and name HG2%)
     3.200     2.600     2.300 peak 29782 weight  0.10000E+01 volume  0.72004E+02 ppm1     4.507 ppm2     1.604
ASSI (29792)
   (( segid "BrD " and resid 27   and name HB1 ))
   (( segid "BrD " and resid 24   and name HB2 ))
     3.400     2.900     2.100 peak 29792 weight  0.10000E+01 volume  0.52302E+02 ppm1     4.607 ppm2     3.077
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OR (29792)
   (( segid "BrD " and resid 27   and name HB1 ))
   (( segid "BrD " and resid 24   and name HG2 ))
ASSI (29832)
   (( segid "BrD " and resid 66   and name HD2 ))
   (( segid "BrD " and resid 65   and name HA  ))
     4.000     4.000     1.500 peak 29832 weight  0.10000E+01 volume  0.19067E+02 ppm1     3.631 ppm2     5.390
ASSI (29842)
   (( segid "BrD " and resid 66   and name HD1 ))
   (( segid "BrD " and resid 65   and name HA  ))
     4.300     4.300     1.200 peak 29842 weight  0.10000E+01 volume  0.12737E+02 ppm1     3.673 ppm2     5.390
ASSI (29852)
   (( segid "BrD " and resid 66   and name HD1 ))
   (  segid "BrD " and resid 15   and name HE% )
     2.800     2.000     2.000 peak 29852 weight  0.10000E+01 volume  0.17551E+03 ppm1     3.673 ppm2     7.488
ASSI (29882)
   (( segid "BrD " and resid 66   and name HD2 ))
   (  segid "BrD " and resid 15   and name HE% )
     2.700     1.800     1.800 peak 29882 weight  0.10000E+01 volume  0.20920E+03 ppm1     3.631 ppm2     7.488
ASSI (29912)
   (( segid "BrD " and resid 66   and name HA  ))
   (( segid "BrD " and resid 65   and name HA  ))
     3.500     3.100     2.000 peak 29912 weight  0.10000E+01 volume  0.40427E+02 ppm1     5.001 ppm2     5.367
ASSI (29922)
   (( segid "BrD " and resid 66   and name HB2 ))
   (( segid "BrD " and resid 65   and name HA  ))
     4.700     4.700     0.800 peak 29922 weight  0.10000E+01 volume  0.75028E+01 ppm1     2.634 ppm2     5.395
ASSI (29982)
   (( segid "BrD " and resid 66   and name HB2 ))
   (  segid "BrD " and resid 69   and name HG1%)
     3.900     3.800     1.600 peak 29982 weight  0.10000E+01 volume  0.21633E+02 ppm1     2.633 ppm2     1.550
ASSI (29992)
   (( segid "BrD " and resid 66   and name HB1 ))
   (  segid "BrD " and resid 69   and name HG1%)
     3.900     3.800     1.600 peak 29992 weight  0.10000E+01 volume  0.22947E+02 ppm1     2.701 ppm2     1.551
ASSI (30022)
   (( segid "BrD " and resid 51   and name HA  ))
   (( segid "BrD " and resid 53   and name HD2 ))
     5.500     5.500     0.000 peak 30022 weight  0.10000E+01 volume  0.72129E-01 ppm1     4.459 ppm2     4.011
ASSI (30062)
   (( segid "BrD " and resid 103  and name HB2 ))
   (( segid "BrD " and resid 82   and name HB1 ))
     3.100     2.400     2.400 peak 30062 weight  0.10000E+01 volume  0.91298E+02 ppm1     1.896 ppm2     3.706
ASSI (30132)
   (( segid "BrD " and resid 116  and name HG11))
   (  segid "BrD " and resid 107  and name HE% )
     2.900     2.100     2.100 peak 30132 weight  0.10000E+01 volume  0.12243E+03 ppm1     1.946 ppm2     7.891
ASSI (30142)
   (( segid "BrD " and resid 116  and name HG11))
   (  segid "BrD " and resid 107  and name HD% )
     3.100     2.400     2.400 peak 30142 weight  0.10000E+01 volume  0.96863E+02 ppm1     1.946 ppm2     7.835
ASSI (30182)
   (( segid "BrD " and resid 64   and name HG1 ))
   (  segid "BrD " and resid 63   and name HD2%)
     3.500     3.100     2.000 peak 30182 weight  0.10000E+01 volume  0.45416E+02 ppm1     2.190 ppm2     1.489
ASSI (30262)
   (( segid "BrD " and resid 86   and name HG1 ))
   (  segid "BrD " and resid 96   and name HD% )
     3.700     3.400     1.800 peak 30262 weight  0.10000E+01 volume  0.30501E+02 ppm1     1.891 ppm2     7.722
ASSI (30322)
   (( segid "BrD " and resid 86   and name HG2 ))
   (( segid "BrD " and resid 87   and name HG1 ))
     3.400     2.900     2.100 peak 30322 weight  0.10000E+01 volume  0.52723E+02 ppm1     0.760 ppm2     3.028
ASSI (30362)
   (( segid "BrD " and resid 103  and name HB2 ))
   (  segid "BrD " and resid 99   and name HB% )
     2.200     1.300     1.300 peak 30362 weight  0.10000E+01 volume  0.49767E+03 ppm1     1.892 ppm2     2.206
ASSI (30422)
   (( segid "BrD " and resid 86   and name HE1 ))
   (  segid "BrD " and resid 99   and name HB% )
     2.500     1.600     1.600 peak 30422 weight  0.10000E+01 volume  0.29716E+03 ppm1     3.078 ppm2     2.206
ASSI (30492)
   (( segid "BrD " and resid 109  and name HE2 ))
   (( segid "BrD " and resid 106  and name HA  ))
     3.000     2.200     2.200 peak 30492 weight  0.10000E+01 volume  0.11643E+03 ppm1     3.029 ppm2     4.591
ASSI (30502)
   (( segid "BrD " and resid 109  and name HE1 ))
   (( segid "BrD " and resid 106  and name HA  ))
     3.800     3.600     1.700 peak 30502 weight  0.10000E+01 volume  0.25593E+02 ppm1     3.177 ppm2     4.590
ASSI (30532)
   (( segid "BrD " and resid 109  and name HD1 ))
   (( segid "BrD " and resid 112  and name HG1 ))
     3.300     2.700     2.200 peak 30532 weight  0.10000E+01 volume  0.67000E+02 ppm1     1.994 ppm2     2.968
ASSI (30682)
   (( segid "BrD " and resid 109  and name HA  ))
   (  segid "BrD " and resid 21   and name HG2%)
     3.600     3.200     1.900 peak 30682 weight  0.10000E+01 volume  0.34166E+02 ppm1     4.656 ppm2     1.588
ASSI (30702)
   (( segid "BrD " and resid 109  and name HA  ))
   (( segid "BrD " and resid 112  and name HG1 ))
     3.800     3.600     1.700 peak 30702 weight  0.10000E+01 volume  0.26014E+02 ppm1     4.653 ppm2     2.964
ASSI (30722)
   (( segid "BrD " and resid 109  and name HA  ))
   (( segid "BrD " and resid 112  and name HG2 ))
     3.200     2.600     2.300 peak 30722 weight  0.10000E+01 volume  0.68767E+02 ppm1     4.653 ppm2     2.823
ASSI (30772)
   (( segid "BrD " and resid 104  and name HB1 ))
   (  segid "BrD " and resid 105  and name HD% )
     3.200     2.600     2.300 peak 30772 weight  0.10000E+01 volume  0.81070E+02 ppm1     2.536 ppm2     7.619
ASSI (30922)
   (( segid "BrD " and resid 19   and name HB1 ))
   (  segid "BrD " and resid 15   and name HE% )
     3.200     2.600     2.300 peak 30922 weight  0.10000E+01 volume  0.75523E+02 ppm1     2.289 ppm2     7.486
ASSI (30962)
   (( segid "BrD " and resid 59   and name HB2 ))
   (( segid "BrD " and resid 56   and name HA  ))
     2.300     1.300     1.300 peak 30962 weight  0.10000E+01 volume  0.51425E+03 ppm1     2.486 ppm2     4.646
ASSI (31062)
   (( segid "BrD " and resid 22   and name HG  ))
   (  segid "BrD " and resid 74   and name HE% )
     2.500     2.500     2.000 peak 31062 weight  0.10000E+01 volume  0.34749E+03 ppm1     2.388 ppm2     7.497
ASSI (31162)
   (( segid "BrD " and resid 54   and name HG1 ))
   (( segid "BrD " and resid 77   and name HA  ))
     3.100     2.600     2.400 peak 31162 weight  0.10000E+01 volume  0.89147E+02 ppm1     3.388 ppm2     4.964
ASSI (   13)
   (  segid "BrD " and resid 46   and name HD% )
   (  segid "BrD " and resid 88   and name HE% )
     2.900     2.100     2.100 peak   13 weight  0.11000E+01 volume  0.62066E+02 ppm1     5.758 ppm2     7.421
ASSI (   23)
   (  segid "BrD " and resid 47   and name HD% )
   (  segid "BrD " and resid 47   and name HE% )
     3.200     2.600     2.300 peak   23 weight  0.11000E+01 volume  0.31210E+02 ppm1     5.758 ppm2     7.261
ASSI (   43)
   (  segid "BrD " and resid 46   and name HE% )
   (  segid "BrD " and resid 88   and name HE% )
     3.800     3.600     1.700 peak   43 weight  0.11000E+01 volume  0.11086E+02 ppm1     6.688 ppm2     7.421
ASSI (   53)
   (  segid "BrD " and resid 46   and name HE% )
   (  segid "BrD " and resid 47   and name HE% )
     4.000     4.000     1.500 peak   53 weight  0.11000E+01 volume  0.78634E+01 ppm1     6.688 ppm2     7.261
ASSI (   93)
   (  segid "BrD " and resid 46   and name HD% )
   (( segid "BrD " and resid 46   and name HA  ))
     2.600     1.700     1.700 peak   93 weight  0.11000E+01 volume  0.11748E+03 ppm1     5.758 ppm2     4.154
ASSI (  103)
   (  segid "BrD " and resid 46   and name HE% )
   (( segid "BrD " and resid 88   and name HB1 ))
     2.200     1.300     1.300 peak  103 weight  0.11000E+01 volume  0.25301E+03 ppm1     6.688 ppm2     3.527
ASSI (  113)
   (  segid "BrD " and resid 46   and name HE% )
   (( segid "BrD " and resid 46   and name HB1 ))
     3.300     2.700     2.200 peak  113 weight  0.11000E+01 volume  0.27341E+02 ppm1     6.688 ppm2     3.279
ASSI (  133)
   (  segid "BrD " and resid 46   and name HD% )
   (( segid "BrD " and resid 46   and name HB2 ))
     2.500     1.600     1.600 peak  133 weight  0.11000E+01 volume  0.14809E+03 ppm1     5.758 ppm2     3.104
ASSI (  153)
   (  segid "BrD " and resid 46   and name HE% )
   (  segid "BrD " and resid 50   and name HD1%)
     3.000     2.200     2.200 peak  153 weight  0.11000E+01 volume  0.42674E+02 ppm1     6.685 ppm2     1.146
ASSI (  273)
   (( segid "BrD " and resid 28   and name HE1 ))
   (( segid "BrD " and resid 28   and name HA  ))
     3.600     3.200     1.900 peak  273 weight  0.11000E+01 volume  0.14248E+02 ppm1     8.129 ppm2     4.533
ASSI (  333)
   (  segid "BrD " and resid 67   and name HD% )
   (  segid "BrD " and resid 68   and name HD% )
     3.000     2.200     2.200 peak  333 weight  0.11000E+01 volume  0.41792E+02 ppm1     6.873 ppm2     7.772
ASSI (  343)
   (  segid "BrD " and resid 67   and name HD% )
   (( segid "BrD " and resid 68   and name HA  ))
     2.800     2.000     2.000 peak  343 weight  0.11000E+01 volume  0.67483E+02 ppm1     6.874 ppm2     5.146
ASSI (  353)
   (  segid "BrD " and resid 67   and name HD% )
   (( segid "BrD " and resid 67   and name HA  ))
     2.500     1.600     1.600 peak  353 weight  0.11000E+01 volume  0.12803E+03 ppm1     6.872 ppm2     4.678
ASSI (  373)
   (  segid "BrD " and resid 67   and name HD% )
   (( segid "BrD " and resid 67   and name HB1 ))
     2.300     1.300     1.300 peak  373 weight  0.11000E+01 volume  0.22980E+03 ppm1     6.874 ppm2     3.570
ASSI (  383)
   (  segid "BrD " and resid 67   and name HE% )
   (  segid "BrD " and resid 68   and name HD% )
     2.900     2.100     2.100 peak  383 weight  0.11000E+01 volume  0.60490E+02 ppm1     7.293 ppm2     7.780
ASSI (  403)
   (  segid "BrD " and resid 67   and name HE% )
   (  segid "BrD " and resid 68   and name HE% )
     2.400     1.400     1.400 peak  403 weight  0.11000E+01 volume  0.16842E+03 ppm1     7.293 ppm2     7.888
ASSI (  433)
   (  segid "BrD " and resid 67   and name HE% )
   (( segid "BrD " and resid 67   and name HA  ))
     3.000     2.200     2.200 peak  433 weight  0.11000E+01 volume  0.50708E+02 ppm1     7.292 ppm2     4.679
ASSI (  463)
   (  segid "BrD " and resid 47   and name HE% )
   (  segid "BrD " and resid 46   and name HD% )
     2.900     2.100     2.100 peak  463 weight  0.11000E+01 volume  0.86184E+02 ppm1     7.246 ppm2     5.744
ASSI (  493)
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   ( segid "BrD " and resid 47   and name HE% )
   (( segid "BrD " and resid 47   and name HA  ))
     3.300     2.700     2.200 peak   493 weight  0.11000E+01 volume  0.27001E+02 ppm1      7.246 ppm2      4.711
ASSI { 503}
   ( segid "BrD " and resid 47   and name HD% )
   (( segid "BrD " and resid 47   and name HA  ))
     2.200     1.200     1.200 peak   503 weight  0.11000E+01 volume  0.29622E+02 ppm1      7.942 ppm2      4.693
ASSI { 543}
   (( segid "BrD " and resid 32   and name HD1 ))
   (( segid "BrD " and resid 30   and name HA  ))
     2.600     1.700     1.700 peak   543 weight  0.11000E+01 volume  0.10449E+02 ppm1      8.455 ppm2      5.452
ASSI { 563}
   (( segid "BrD " and resid 32   and name HD1 ))
   (( segid "BrD " and resid 32   and name HB2 ))
     2.900     2.100     2.100 peak   563 weight  0.11000E+01 volume  0.53265E+02 ppm1      8.456 ppm2      3.942
ASSI { 603}
   ( segid "BrD " and resid 74   and name HD% )
   (( segid "BrD " and resid 74   and name HA  ))
     2.500     1.600     1.600 peak   603 weight  0.11000E+01 volume  0.15470E+03 ppm1      7.013 ppm2      4.373
ASSI { 843}
   ( segid "BrD " and resid 15   and name HD% )
   (( segid "BrD " and resid 15   and name HA  ))
     1.900     0.900     0.900 peak   843 weight  0.11000E+01 volume  0.61725E+03 ppm1      7.664 ppm2      4.621
ASSI { 863}
   ( segid "BrD " and resid 15   and name HD% )
   (( segid "BrD " and resid 15   and name HB1 ))
     2.400     1.400     1.400 peak   863 weight  0.11000E+01 volume  0.19360E+03 ppm1      7.664 ppm2      3.818
ASSI { 873}
   ( segid "BrD " and resid 15   and name HD% )
   (( segid "BrD " and resid 15   and name HB2 ))
     2.000     1.000     1.000 peak   873 weight  0.11000E+01 volume  0.48925E+03 ppm1      7.664 ppm2      3.643
ASSI { 893}
   ( segid "BrD " and resid 15   and name HE% )
   (( segid "BrD " and resid 15   and name HA  ))
     3.500     3.100     2.000 peak   893 weight  0.11000E+01 volume  0.17907E+02 ppm1      7.478 ppm2      4.635
ASSI { 903}
   ( segid "BrD " and resid 15   and name HE% )
   (( segid "BrD " and resid 15   and name HB2 ))
     4.000     4.000     1.500 peak   903 weight  0.11000E+01 volume  0.77515E+01 ppm1      7.478 ppm2      3.643
ASSI { 993}
   ( segid "BrD " and resid 68   and name HE% )
   ( segid "BrD " and resid 74   and name HD% )
     3.100     2.400     2.400 peak   993 weight  0.11000E+01 volume  0.39808E+02 ppm1      7.850 ppm2      6.998
ASSI { 1003}
   ( segid "BrD " and resid 68   and name HE% )
   ( segid "BrD " and resid 67   and name HD% )
     2.900     2.100     2.100 peak  1003 weight  0.11000E+01 volume  0.57511E+02 ppm1      7.850 ppm2      6.896
ASSI { 1063}
   ( segid "BrD " and resid 68   and name HE% )
   (( segid "BrD " and resid 68   and name HA  ))
     2.900     2.100     2.100 peak  1063 weight  0.11000E+01 volume  0.51154E+02 ppm1      7.850 ppm2      5.146
ASSI { 1213}
   ( segid "BrD " and resid 68   and name HD% )
   (( segid "BrD " and resid 68   and name HB1 ))
     2.000     1.000     1.000 peak  1213 weight  0.11000E+01 volume  0.59736E+03 ppm1      7.757 ppm2      3.673
ASSI { 1263}
   ( segid "BrD " and resid 88   and name HD% )
   ( segid "BrD " and resid 46   and name HE% )
     2.800     2.000     2.000 peak  1263 weight  0.11000E+01 volume  0.62764E+02 ppm1      7.618 ppm2      6.692
ASSI { 1283}
   ( segid "BrD " and resid 88   and name HD% )
   ( segid "BrD " and resid 46   and name HD% )
     3.100     2.400     2.400 peak  1283 weight  0.11000E+01 volume  0.38726E+02 ppm1      7.616 ppm2      5.745
ASSI { 1303}
   ( segid "BrD " and resid 88   and name HD% )
   (( segid "BrD " and resid 88   and name HA  ))
     2.200     1.200     1.200 peak  1303 weight  0.11000E+01 volume  0.31179E+03 ppm1      7.616 ppm2      4.999
ASSI { 1313}
   ( segid "BrD " and resid 88   and name HE% )
   (( segid "BrD " and resid 88   and name HA  ))
     2.800     2.000     2.000 peak  1313 weight  0.11000E+01 volume  0.64049E+02 ppm1      7.410 ppm2      4.999
ASSI { 1323}
   ( segid "BrD " and resid 88   and name HD% )
   (( segid "BrD " and resid 46   and name HA  ))
     3.100     2.400     2.400 peak  1323 weight  0.11000E+01 volume  0.38562E+02 ppm1      7.618 ppm2      4.154
ASSI { 1363}
   ( segid "BrD " and resid 88   and name HD% )
   (( segid "BrD " and resid 88   and name HB1 ))
     2.300     1.300     1.300 peak  1363 weight  0.11000E+01 volume  0.21010E+03 ppm1      7.616 ppm2      3.531
ASSI { 1403}
   ( segid "BrD " and resid 96   and name HD% )
   (( segid "BrD " and resid 96   and name HA  ))
     2.400     1.400     1.400 peak  1403 weight  0.11000E+01 volume  0.18299E+03 ppm1      7.711 ppm2      4.431
ASSI { 1413}
   ( segid "BrD " and resid 96   and name HD% )
   (( segid "BrD " and resid 96   and name HB1 ))
     2.400     1.400     1.400 peak  1413 weight  0.11000E+01 volume  0.19687E+03 ppm1      7.712 ppm2      3.896
ASSI { 1503}
   ( segid "BrD " and resid 34   and name HD% )
   (( segid "BrD " and resid 31   and name HA  ))
     3.200     1.200     1.200 peak  1503 weight  0.11000E+01 volume  0.28381E+03 ppm1      7.708 ppm2      4.985
ASSI { 1583}
   ( segid "BrD " and resid 107  and name HE% )
   (( segid "BrD " and resid 107  and name HB1 ))
     3.200     2.600     2.300 peak  1583 weight  0.11000E+01 volume  0.29123E+02 ppm1      7.896 ppm2      3.674
ASSI { 1793}
   ( segid "BrD " and resid 95   and name HD% )
   (( segid "BrD " and resid 95   and name HB2 ))
     3.400     2.900     2.100 peak  1793 weight  0.11000E+01 volume  0.22641E+02 ppm1      7.478 ppm2      3.352
ASSI { 1833}
   ( segid "BrD " and resid 95   and name HD% )
   (( segid "BrD " and resid 95   and name HA  ))
     2.100     1.100     1.100 peak  1833 weight  0.11000E+01 volume  0.35285E+03 ppm1      7.478 ppm2      4.446
ASSI { 1883}
   ( segid "BrD " and resid 95   and name HE% )
   (( segid "BrD " and resid 95   and name HA  ))
     3.400     2.900     2.100 peak  1883 weight  0.11000E+01 volume  0.23591E+02 ppm1      7.617 ppm2      4.446
ASSI { 1943}
   ( segid "BrD " and resid 95   and name HE% )
   (( segid "BrD " and resid 32   and name HN2 ))
     1.800     0.800     0.800 peak  1943 weight  0.11000E+01 volume  0.97461E+03 ppm1      7.619 ppm2      7.785
ASSI { 1963}
   ( segid "BrD " and resid 95   and name HE% )
   (( segid "BrD " and resid 32   and name HZ2 ))
     3.400     2.900     2.100 peak  1963 weight  0.11000E+01 volume  0.21009E+02 ppm1      7.618 ppm2      8.002
ASSI { 2023}
   (( segid "BrD " and resid 32   and name HN2 ))
   (( segid "BrD " and resid 32   and name HZ2 ))
     2.100     1.100     1.100 peak  2023 weight  0.11000E+01 volume  0.40155E+03 ppm1      7.757 ppm2      8.004
ASSI { 2133}
   (( segid "BrD " and resid 82   and name HZ  ))
   ( segid "BrD " and resid 82   and name HD% )
     2.600     1.700     1.700 peak  2133 weight  0.11000E+01 volume  0.10557E+03 ppm1      7.013 ppm2      7.261
ASSI { 163}
   ( segid "BrD " and resid 46   and name HE% )
   ( segid "BrD " and resid 38   and name HG1% )
     3.000     2.200     2.200 peak   163 weight  0.10000E+01 volume  0.48608E+02 ppm1      6.668 ppm2      1.076
ASSI { 183}
   ( segid "BrD " and resid 46   and name HD% )
   (( segid "BrD " and resid 50   and name HB  ))
     3.100     2.400     2.400 peak   183 weight  0.10000E+01 volume  0.36832E+02 ppm1      5.758 ppm2      1.791
ASSI { 253}
   (( segid "BrD " and resid 28   and name HE1 ))
   ( segid "BrD " and resid 101  and name HG2% )
     2.800     2.000     2.000 peak   253 weight  0.10000E+01 volume  0.66486E+02 ppm1      8.130 ppm2      1.601
ASSI { 263}
   (( segid "BrD " and resid 28   and name HE1 ))
   ( segid "BrD " and resid 101  and name HD1% )
     2.600     1.700     1.700 peak   263 weight  0.10000E+01 volume  0.12057E+03 ppm1      8.129 ppm2      1.528
ASSI { 283}
   (( segid "BrD " and resid 28   and name HE1 ))
   (( segid "BrD " and resid 30   and name HB1 ))
     2.900     2.100     2.100 peak   283 weight  0.10000E+01 volume  0.53269E+02 ppm1      8.129 ppm2      4.927
ASSI { 733}
   ( segid "BrD " and resid 74   and name HE% )
   ( segid "BrD " and resid 63   and name HD1% )
     3.700     3.400     1.800 peak   733 weight  0.10000E+01 volume  0.13584E+02 ppm1      7.524 ppm2      1.704
ASSI { 793}
   ( segid "BrD " and resid 82   and name HE% )
   ( segid "BrD " and resid 106  and name HD% )
     3.500     3.100     2.000 peak   793 weight  0.10000E+01 volume  0.18520E+02 ppm1      7.060 ppm2      7.494
ASSI { 1113}
   ( segid "BrD " and resid 68   and name HD% )
   (( segid "BrD " and resid 62   and name HD2 ))
     2.600     1.700     1.700 peak  1113 weight  0.10000E+01 volume  0.11215E+03 ppm1      7.758 ppm2      2.595
ASSI { 1133}
   ( segid "BrD " and resid 68   and name HD% )
   (( segid "BrD " and resid 62   and name HB2 ))
     2.600     2.000     2.000 peak  1133 weight  0.10000E+01 volume  0.66543E+02 ppm1      7.757 ppm2      1.718
ASSI { 1173}
   ( segid "BrD " and resid 105  and name HD% )
   ( segid "BrD " and resid 102  and name HD2% )
     2.800     2.000     2.000 peak  1173 weight  0.10000E+01 volume  0.71257E+02 ppm1      7.758 ppm2      1.338
OR { 1173}
   ( segid "BrD " and resid 105  and name HD% )
   ( segid "BrD " and resid 102  and name HD1% )
ASSI { 1353}
   ( segid "BrD " and resid 88   and name HE% )
   (( segid "BrD " and resid 88   and name HB1 ))
     3.400     2.900     2.100 peak  1353 weight  0.10000E+01 volume  0.21121E+02 ppm1      7.413 ppm2      3.527
ASSI { 1423}
   ( segid "BrD " and resid 96   and name HD% )
   (( segid "BrD " and resid 100  and name HB1 ))
     3.100     2.400     2.400 peak  1423 weight  0.10000E+01 volume  0.40018E+02 ppm1      7.711 ppm2      3.454
OR { 1423}
   ( segid "BrD " and resid 96   and name HD% )
   (( segid "BrD " and resid 100  and name HB2 ))
ASSI { 1613}
   ( segid "BrD " and resid 107  and name HD% )
   (( segid "BrD " and resid 106  and name HB1 ))
     3.600     3.200     1.900 peak  1613 weight  0.10000E+01 volume  0.14818E+02 ppm1      7.803 ppm2      3.953
ASSI { 1663}
   ( segid "BrD " and resid 107  and name HD% )
   (( segid "BrD " and resid 103  and name HA  ))
     3.100     2.400     2.400 peak  1663 weight  0.10000E+01 volume  0.38863E+02 ppm1      7.803 ppm2      3.804
ASSI { 1753}
   ( segid "BrD " and resid 106  and name HE% )
   (( segid "BrD " and resid 75   and name HA  ))
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    3.700     3.400     1.800 peak  1753 weight  0.10000E+01 volume  0.13649E+02 ppm1      7.617 ppm2      4.534
ASSI [ 1803]
  ( segid "BrD " and resid 95   and name HD% )
  (( segid "BrD " and resid 65   and name HA  ))
    3.300     2.700     2.200 peak  1803 weight  0.10000E+01 volume  0.27238E+02 ppm1      7.478 ppm2      4.985
ASSI [ 1853]
  ( segid "BrD " and resid 95   and name HD% )
  (( segid "BrD " and resid 65   and name HB1 ))
    3.300     2.700     2.200 peak  1853 weight  0.10000E+01 volume  0.27537E+02 ppm1      7.479 ppm2      3.920
ASSI [ 1863]
  ( segid "BrD " and resid 95   and name HD% )
  (( segid "BrD " and resid 33   and name HB1 ))
    3.200     2.600     2.300 peak  1863 weight  0.10000E+01 volume  0.30330E+02 ppm1      7.478 ppm2      1.047
ASSI [ 1903]
  ( segid "BrD " and resid 95   and name HE% )
  (( segid "BrD " and resid 33   and name HA  ))
    3.500     3.100     2.000 peak  1903 weight  0.10000E+01 volume  0.17985E+02 ppm1      7.618 ppm2      4.343
ASSI [ 2003]
  (( segid "BrD " and resid 32   and name HH2 ))
  ( segid "BrD " and resid 95   and name HD% )
    4.300     4.300     1.200 peak  2003 weight  0.10000E+01 volume  0.52192E+01 ppm1      7.757 ppm2      7.509
ASSI [ 2143]
  (( segid "BrD " and resid 62   and name HZ  ))
  ( segid "BrD " and resid 106  and name HD% )
    3.800     3.600     1.700 peak  2143 weight  0.10000E+01 volume  0.11127E+02 ppm1      7.013 ppm2      7.509
ASSI [ 2183]
  ( segid "BrD " and resid 107  and name HE% )
  (( segid "BrD " and resid 79   and name HG1 ))
    3.500     3.100     2.000 peak  2183 weight  0.10000E+01 volume  0.19805E+02 ppm1      7.897 ppm2      3.060
ASSI [   54]
  ( segid "BrD " and resid 47   and name HD% )
  (( segid "BrD " and resid 47   and name HB1 ))
    2.200     1.200     1.200 peak    54 weight  0.10000E+01 volume  0.95156E+03 ppm1      7.970 ppm2      1.806
ASSI [   64]
  ( segid "BrD " and resid 47   and name HD% )
  (( segid "BrD " and resid 47   and name HB2 ))
    2.300     1.300     1.300 peak    64 weight  0.10000E+01 volume  0.78671E+03 ppm1      7.970 ppm2      3.415
ASSI [  144]
  ( segid "BrD " and resid 67   and name HD% )
  ( segid "BrD " and resid 67   and name HE% )
    2.000     1.000     1.000 peak   144 weight  0.10000E+01 volume  0.18744E+04 ppm1      6.900 ppm2      7.321
ASSI [  214]
  ( segid "BrD " and resid 67   and name HD% )
  (( segid "BrD " and resid 67   and name HB2 ))
    2.200     1.200     1.200 peak   214 weight  0.10000E+01 volume  0.10973E+04 ppm1      6.899 ppm2      2.664
ASSI [  274]
  ( segid "BrD " and resid 68   and name HD% )
  (( segid "BrD " and resid 68   and name HA  ))
    2.400     1.400     1.400 peak   274 weight  0.10000E+01 volume  0.56412E+03 ppm1      7.778 ppm2      5.140
ASSI [  294]
  ( segid "BrD " and resid 68   and name HD% )
  (( segid "BrD " and resid 68   and name HB2 ))
    2.300     1.300     1.300 peak   294 weight  0.10000E+01 volume  0.81340E+03 ppm1      7.778 ppm2      3.546
ASSI [  354]
  ( segid "BrD " and resid 88   and name HD% )
  ( segid "BrD " and resid 88   and name HE% )
    2.000     1.000     1.000 peak   354 weight  0.10000E+01 volume  0.17752E+04 ppm1      7.612 ppm2      7.418
ASSI [  454]
  (( segid "BrD " and resid 32   and name HD1 ))
  (( segid "BrD " and resid 32   and name HA  ))
    3.000     2.200     2.200 peak   454 weight  0.10000E+01 volume  0.17821E+03 ppm1      8.491 ppm2      4.977
ASSI [  474]
  (( segid "BrD " and resid 32   and name HD1 ))
  (( segid "BrD " and resid 32   and name HB1 ))
    3.100     2.400     2.400 peak   474 weight  0.10000E+01 volume  0.14234E+03 ppm1      8.490 ppm2      4.213
ASSI [ 1694]
  ( segid "BrD " and resid 34   and name HE% )
  (( segid "BrD " and resid 34   and name HB1 ))
    3.300     2.700     2.200 peak  1694 weight  0.10000E+01 volume  0.91431E+02 ppm1      7.781 ppm2      4.116
ASSI [ 1834]
  ( segid "BrD " and resid 96   and name HD% )
  ( segid "BrD " and resid 96   and name HE% )
    1.900     0.900     0.900 peak  1834 weight  0.10000E+01 volume  0.29744E+04 ppm1      7.724 ppm2      7.614
ASSI [ 1914]
  ( segid "BrD " and resid 96   and name HD% )
  (( segid "BrD " and resid 96   and name HB2 ))
    2.200     1.200     1.200 peak  1914 weight  0.10000E+01 volume  0.99570E+03 ppm1      7.726 ppm2      3.124
ASSI [ 2024]
  ( segid "BrD " and resid 34   and name HD% )
  (( segid "BrD " and resid 34   and name HB1 ))
    2.500     1.600     1.600 peak  2024 weight  0.10000E+01 volume  0.48715E+03 ppm1      7.714 ppm2      4.115
ASSI [ 2084]
  ( segid "BrD " and resid 15   and name HD% )
  ( segid "BrD " and resid 15   and name HE% )
    1.900     0.900     0.900 peak  2084 weight  0.10000E+01 volume  0.28924E+04 ppm1      7.689 ppm2      7.483
ASSI [ 2474]
  ( segid "BrD " and resid 96   and name HE% )
  (( segid "BrD " and resid 96   and name HB1 ))
    3.300     2.700     2.200 peak  2474 weight  0.10000E+01 volume  0.86809E+02 ppm1      7.611 ppm2      4.001
ASSI [ 2554]
  ( segid "BrD " and resid 74   and name HE% )
  ( segid "BrD " and resid 74   and name HD% )
    2.000     1.000     1.000 peak  2554 weight  0.10000E+01 volume  0.18278E+04 ppm1      7.539 ppm2      7.006
ASSI [ 3204]
  ( segid "BrD " and resid 82   and name HD% )
  (( segid "BrD " and resid 82   and name HB1 ))
    2.400     1.400     1.400 peak  3204 weight  0.10000E+01 volume  0.67788E+03 ppm1      7.265 ppm2      3.708
ASSI [ 3214]
  ( segid "BrD " and resid 82   and name HD% )
  (( segid "BrD " and resid 82   and name HB2 ))
    2.300     1.300     1.300 peak  3214 weight  0.10000E+01 volume  0.77298E+03 ppm1      7.262 ppm2      3.571
ASSI [ 3304]
  ( segid "BrD " and resid 82   and name HD% )
  ( segid "BrD " and resid 82   and name HE% )
    2.100     1.100     1.100 peak  3304 weight  0.10000E+01 volume  0.12642E+04 ppm1      7.262 ppm2      7.076
ASSI [ 3644]
  ( segid "BrD " and resid 74   and name HD% )
  (( segid "BrD " and resid 74   and name HB2 ))
    2.400     1.400     1.400 peak  3644 weight  0.10000E+01 volume  0.64123E+03 ppm1      7.005 ppm2      3.007
ASSI [ 3894]
  ( segid "BrD " and resid 46   and name HD% )
  ( segid "BrD " and resid 46   and name HE% )
    2.000     1.000     1.000 peak  3894 weight  0.10000E+01 volume  0.17599E+04 ppm1      5.743 ppm2      6.687
ASSI [ 3914]
  ( segid "BrD " and resid 46   and name HD% )
  (( segid "BrD " and resid 46   and name HB1 ))
    2.400     1.400     1.400 peak  3914 weight  0.10000E+01 volume  0.61947E+03 ppm1      5.740 ppm2      3.304
ASSI [ 4064]
  (( segid "BrD " and resid 28   and name HD2 ))
  (( segid "BrD " and resid 28   and name HA  ))
    3.000     2.200     2.200 peak  4064 weight  0.10000E+01 volume  0.15484E+03 ppm1      5.577 ppm2      4.586
ASSI [   84]
  ( segid "BrD " and resid 82   and name HD% )
  (( segid "BrD " and resid 103  and name HA  ))
    2.900     2.100     2.100 peak    84 weight  0.10000E+01 volume  0.22432E+03 ppm1      7.265 ppm2      3.790
ASSI [  174]
  ( segid "BrD " and resid 67   and name HD% )
  (( segid "BrD " and resid 62   and name HA  ))
    3.300     2.700     2.200 peak   174 weight  0.10000E+01 volume  0.89209E+02 ppm1      6.899 ppm2      4.490
ASSI [  244]
  ( segid "BrD " and resid 67   and name HD% )
  (( segid "BrD " and resid 62   and name HB2 ))
    2.900     2.100     2.100 peak   244 weight  0.10000E+01 volume  0.21286E+03 ppm1      6.899 ppm2      1.706
ASSI [  254]
  ( segid "BrD " and resid 67   and name HD% )
  ( segid "BrD " and resid 73   and name HD1% )
    3.500     3.100     2.000 peak   254 weight  0.10000E+01 volume  0.64742E+02 ppm1      6.899 ppm2      1.545
ASSI [  464]
  (( segid "BrD " and resid 32   and name HD1 ))
  (( segid "BrD " and resid 29   and name HA  ))
    3.300     2.700     2.200 peak   464 weight  0.10000E+01 volume  0.97341E+02 ppm1      8.490 ppm2      4.814
ASSI [  494]
  (( segid "BrD " and resid 32   and name HD1 ))
  (( segid "BrD " and resid 33   and name HD1 ))
    5.500     5.500     0.000 peak   494 weight  0.10000E+01 volume  0.38880E-03 ppm1      8.490 ppm2      2.781
ASSI [  504]
  (( segid "BrD " and resid 32   and name HD1 ))
  (( segid "BrD " and resid 33   and name HD2 ))
    4.000     4.000     1.500 peak   504 weight  0.10000E+01 volume  0.30117E+02 ppm1      8.490 ppm2      2.211
ASSI [  564]
  (( segid "BrD " and resid 107  and name HZ  ))
  (( segid "BrD " and resid 79   and name HB1 ))
    3.100     2.400     2.400 peak   564 weight  0.10000E+01 volume  0.14239E+03 ppm1      8.008 ppm2      2.802
ASSI [  624]
  (( segid "BrD " and resid 107  and name HZ  ))
  (( segid "BrD " and resid 79   and name HA  ))
    3.000     2.200     2.200 peak   624 weight  0.10000E+01 volume  0.17938E+03 ppm1      8.058 ppm2      4.439
ASSI [  634]
  (( segid "BrD " and resid 107  and name HZ  ))
  ( segid "BrD " and resid 107  and name HE% )
    2.000     1.000     1.000 peak   634 weight  0.10000E+01 volume  0.19583E+04 ppm1      8.058 ppm2      7.927
ASSI [  644]
  (( segid "BrD " and resid 107  and name HZ  ))
  ( segid "BrD " and resid 107  and name HD% )
    2.500     2.500     2.000 peak   644 weight  0.10000E+01 volume  0.49678E+03 ppm1      8.058 ppm2      7.793
ASSI [  664]
  (( segid "BrD " and resid 107  and name HZ  ))
  (( segid "BrD " and resid 79   and name HG1 ))
    2.700     1.800     1.800 peak   664 weight  0.10000E+01 volume  0.34018E+03 ppm1      8.059 ppm2      2.994
ASSI [  694]
  (( segid "BrD " and resid 32   and name HZ2 ))
  (( segid "BrD " and resid 94   and name HG1 ))
    2.500     1.600     1.600 peak   694 weight  0.10000E+01 volume  0.45123E+03 ppm1      8.008 ppm2      3.154
ASSI [  714]
  (( segid "BrD " and resid 32   and name HZ2 ))
  (( segid "BrD " and resid 32   and name HZ3 ))
    2.100     2.100     2.400 peak   714 weight  0.10000E+01 volume  0.13157E+04 ppm1      8.004 ppm2      7.797
ASSI [  724]
  (( segid "BrD " and resid 32   and name HZ3 ))
  (( segid "BrD " and resid 33   and name HG2 ))
    3.200     2.600     2.300 peak   724 weight  0.10000E+01 volume  0.11962E+03 ppm1      7.959 ppm2     -0.311
ASSI [  804]
  (( segid "BrD " and resid 32   and name HZ2 ))
  (( segid "BrD " and resid 97   and name HB1 ))
    2.700     1.800     1.800 peak   804 weight  0.10000E+01 volume  0.29399E+03 ppm1      7.961 ppm2      2.667
ASSI [  854]
  (( segid "BrD " and resid 32   and name HZ3 ))
  (( segid "BrD " and resid 32   and name HA  ))
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    2.900     2.100     2.100 peak   854 weight  0.10000E+01 volume  0.19220E+03 ppm1      7.957 ppm2      4.976
ASSI [  864]
  (( segid "BrD " and resid 32    and name HE3 ))
  (( segid "BrD " and resid 33    and name HA  ))
    2.600     1.700     1.700 peak   864 weight  0.10000E+01 volume  0.35337E+03 ppm1      7.956 ppm2      4.361
ASSI [  874]
  (( segid "BrD " and resid 32    and name HE3 ))
  (( segid "BrD " and resid 32    and name HB1 ))
    2.800     2.000     2.000 peak   874 weight  0.10000E+01 volume  0.24269E+03 ppm1      7.958 ppm2      3.966
ASSI [  984]
  (  segid "BrD " and resid 107   and name HE% )
  (( segid "BrD " and resid 103   and name HA  ))
    3.000     2.200     2.200 peak   984 weight  0.10000E+01 volume  0.17386E+03 ppm1      7.925 ppm2      3.742
ASSI [ 1024]
  (( segid "BrD " and resid 34    and name HZ  ))
  (( segid "BrD " and resid 102   and name HB2 ))
    2.500     1.600     1.600 peak  1024 weight  0.10000E+01 volume  0.46463E+03 ppm1      7.926 ppm2      1.813
ASSI [ 1144]
  (( segid "BrD " and resid 34    and name HZ  ))
  (( segid "BrD " and resid 102   and name HB1 ))
    2.900     2.100     2.100 peak  1144 weight  0.10000E+01 volume  0.21471E+03 ppm1      7.900 ppm2      1.967
ASSI [ 1154]
  (( segid "BrD " and resid 34    and name HZ  ))
  (( segid "BrD " and resid 98    and name HB1 ))
    3.300     2.700     2.200 peak  1154 weight  0.10000E+01 volume  0.95962E+02 ppm1      7.899 ppm2      4.001
ASSI [ 1194]
  (  segid "BrD " and resid 107   and name HE% )
  (( segid "BrD " and resid 79    and name HA  ))
    2.300     1.300     1.300 peak  1194 weight  0.10000E+01 volume  0.84240E+03 ppm1      7.889 ppm2      4.391
ASSI [ 1224]
  (  segid "BrD " and resid 68    and name HE% )
  (( segid "BrD " and resid 62    and name HD1 ))
    3.100     2.400     2.400 peak  1224 weight  0.10000E+01 volume  0.13020E+03 ppm1      7.892 ppm2      3.172
ASSI [ 1314]
  (  segid "BrD " and resid 68    and name HE% )
  (  segid "BrD " and resid 73    and name HD2% )
    4.100     4.100     1.400 peak  1314 weight  0.10000E+01 volume  0.23932E+02 ppm1      7.892 ppm2      1.496
ASSI [ 1344]
  (( segid "BrD " and resid 32    and name HE3 ))
  (( segid "BrD " and resid 33    and name HD2 ))
    3.200     2.600     2.300 peak  1344 weight  0.10000E+01 volume  0.10782E+03 ppm1      7.956 ppm2      2.212
ASSI [ 1434]
  (( segid "BrD " and resid 32    and name HZ3 ))
  (( segid "BrD " and resid 32    and name HE3 ))
    1.800     0.800     0.800 peak  1434 weight  0.10000E+01 volume  0.39856E+04 ppm1      7.812 ppm2      7.954
ASSI [ 1454]
  (  segid "BrD " and resid 34    and name HE% )
  (  segid "BrD " and resid 102   and name HD1% )
    2.900     2.100     2.100 peak  1454 weight  0.10000E+01 volume  0.19468E+03 ppm1      7.808 ppm2      1.268
ASSI [ 1464]
  (  segid "BrD " and resid 107   and name HD% )
  (  segid "BrD " and resid 110   and name HD1% )
    2.800     2.000     2.000 peak  1464 weight  0.10000E+01 volume  0.23444E+03 ppm1      7.810 ppm2      1.153
ASSI [ 1474]
  (  segid "BrD " and resid 107   and name HD% )
  (  segid "BrD " and resid 116   and name HD1% )
    2.600     1.700     1.700 peak  1474 weight  0.10000E+01 volume  0.36349E+03 ppm1      7.806 ppm2      1.399
ASSI [ 1494]
  (  segid "BrD " and resid 107   and name HD% )
  (( segid "BrD " and resid 107   and name HA  ))
    3.300     1.300     1.300 peak  1494 weight  0.10000E+01 volume  0.85611E+03 ppm1      7.803 ppm2      4.440
ASSI [ 1524]
  (  segid "BrD " and resid 105   and name HD% )
  (( segid "BrD " and resid 105   and name HB1 ))
    2.300     1.300     1.300 peak  1524 weight  0.10000E+01 volume  0.86322E+03 ppm1      7.798 ppm2      3.741
ASSI [ 1564]
  (  segid "BrD " and resid 34    and name HE% )
  (( segid "BrD " and resid 28    and name HD2 ))
    3.000     2.200     2.200 peak  1564 weight  0.10000E+01 volume  0.16881E+03 ppm1      7.794 ppm2      5.562
ASSI [ 1594]
  (( segid "BrD " and resid 32    and name HZ3 ))
  (  segid "BrD " and resid 95    and name HE% )
    2.600     1.700     1.700 peak  1594 weight  0.10000E+01 volume  0.36507E+03 ppm1      7.791 ppm2      7.630
ASSI [ 1634]
  (  segid "BrD " and resid 34    and name HE% )
  (( segid "BrD " and resid 102   and name HB1 ))
    3.200     2.600     2.300 peak  1634 weight  0.10000E+01 volume  0.12088E+03 ppm1      7.790 ppm2      2.032
ASSI [ 1644]
  (  segid "BrD " and resid 34    and name HE% )
  (( segid "BrD " and resid 98    and name HB1 ))
    2.700     1.800     1.800 peak  1644 weight  0.10000E+01 volume  0.32157E+03 ppm1      7.784 ppm2      4.016
ASSI [ 1724]
  (  segid "BrD " and resid 107   and name HD% )
  (( segid "BrD " and resid 103   and name HG2 ))
    2.400     2.400     2.100 peak  1724 weight  0.10000E+01 volume  0.57446E+03 ppm1      7.778 ppm2      2.487
ASSI [ 1754]
  (( segid "BrD " and resid 32    and name HZ3 ))
  (( segid "BrD " and resid 33    and name HB1 ))
    2.700     1.800     1.800 peak  1754 weight  0.10000E+01 volume  0.30103E+03 ppm1      7.780 ppm2      1.088
ASSI [ 1764]
  (  segid "BrD " and resid 34    and name HE% )
  (  segid "BrD " and resid 81    and name HG2% )
    3.000     2.200     2.200 peak  1764 weight  0.10000E+01 volume  0.16442E+03 ppm1      7.781 ppm2      0.762
ASSI [ 1794]
  (  segid "BrD " and resid 68    and name HD% )
  (  segid "BrD " and resid 73    and name HD1% )
    2.600     1.700     1.700 peak  1794 weight  0.10000E+01 volume  0.42209E+03 ppm1      7.781 ppm2      1.543
ASSI [ 1904]
  (  segid "BrD " and resid 34    and name HD% )
  (( segid "BrD " and resid 34    and name HZ  ))
    2.600     1.700     1.700 peak  1904 weight  0.10000E+01 volume  0.35620E+03 ppm1      7.719 ppm2      7.901
ASSI [ 1954]
  (  segid "BrD " and resid 34    and name HD% )
  (( segid "BrD " and resid 85    and name HB1 ))
    3.000     2.200     2.200 peak  1954 weight  0.10000E+01 volume  0.18188E+03 ppm1      7.714 ppm2      3.920
ASSI [ 2124]
  (  segid "BrD " and resid 15    and name HD% )
  (  segid "BrD " and resid 63    and name HD1% )
    2.500     1.600     1.600 peak  2124 weight  0.10000E+01 volume  0.44171E+03 ppm1      7.689 ppm2      1.641
ASSI [ 2164]
  (  segid "BrD " and resid 15    and name HD% )
  (( segid "BrD " and resid 16    and name HA  ))
    2.600     1.700     1.700 peak  2164 weight  0.10000E+01 volume  0.41516E+03 ppm1      7.650 ppm2      4.538
ASSI [ 2224]
  (  segid "BrD " and resid 106   and name HE% )
  (  segid "BrD " and resid 75    and name HE% )
    3.000     2.200     2.200 peak  2224 weight  0.10000E+01 volume  0.17361E+03 ppm1      7.646 ppm2      2.666
ASSI [ 2234]
  (  segid "BrD " and resid 106   and name HE% )
  (( segid "BrD " and resid 78    and name HB1 ))
    2.900     2.100     2.100 peak  2234 weight  0.10000E+01 volume  0.21480E+03 ppm1      7.647 ppm2      1.333
ASSI [ 2244]
  (  segid "BrD " and resid 106   and name HE% )
  (( segid "BrD " and resid 78    and name HB1 ))
    2.600     1.700     1.700 peak  2244 weight  0.10000E+01 volume  0.42178E+03 ppm1      7.647 ppm2      1.268
OR [ 2244]
  (  segid "BrD " and resid 106   and name HE% )
  (( segid "BrD " and resid 78    and name HG  ))
ASSI [ 2264]
  (  segid "BrD " and resid 106   and name HE% )
  (( segid "BrD " and resid 106   and name HB1 ))
    2.400     2.900     2.100 peak  2264 weight  0.10000E+01 volume  0.80420E+02 ppm1      7.644 ppm2      3.919
ASSI [ 2414]
  (  segid "BrD " and resid 106   and name HE% )
  (  segid "BrD " and resid 17    and name HG2% )
    4.000     4.000     1.500 peak  2414 weight  0.10000E+01 volume  0.29483E+02 ppm1      7.616 ppm2      1.706
ASSI [ 2484]
  (  segid "BrD " and resid 96    and name HE% )
  (( segid "BrD " and resid 86    and name HE1 ))
    3.000     2.200     2.200 peak  2484 weight  0.10000E+01 volume  0.16268E+03 ppm1      7.611 ppm2      3.106
ASSI [ 2504]
  (  segid "BrD " and resid 106   and name HE% )
  (( segid "BrD " and resid 21    and name HG11))
    2.500     1.600     1.600 peak  2504 weight  0.10000E+01 volume  0.54543E+03 ppm1      7.611 ppm2      2.374
ASSI [ 2514]
  (  segid "BrD " and resid 106   and name HE% )
  (( segid "BrD " and resid 18    and name HG  ))
    2.600     1.700     1.700 peak  2514 weight  0.10000E+01 volume  0.40048E+03 ppm1      7.611 ppm2      2.274
ASSI [ 2574]
  (  segid "BrD " and resid 74    and name HE% )
  (  segid "BrD " and resid 63    and name HD2% )
    2.900     2.100     2.100 peak  2574 weight  0.10000E+01 volume  0.18991E+03 ppm1      7.539 ppm2      1.496
ASSI [ 2614]
  (  segid "BrD " and resid 106   and name HD% )
  (( segid "BrD " and resid 21    and name HG11))
    3.200     2.600     2.300 peak  2614 weight  0.10000E+01 volume  0.10679E+03 ppm1      7.535 ppm2      2.308
ASSI [ 2654]
  (  segid "BrD " and resid 106   and name HD% )
  (  segid "BrD " and resid 21    and name HG2% )
    2.000     1.000     1.000 peak  2654 weight  0.10000E+01 volume  0.21619E+04 ppm1      7.541 ppm2      1.580
ASSI [ 2674]
  (  segid "BrD " and resid 74    and name HE% )
  (( segid "BrD " and resid 78    and name HG  ))
    2.500     1.600     1.600 peak  2674 weight  0.10000E+01 volume  0.54850E+03 ppm1      7.529 ppm2      1.266
ASSI [ 2694]
  (  segid "BrD " and resid 74    and name HE% )
  (  segid "BrD " and resid 78    and name HD1% )
    2.500     1.600     1.600 peak  2694 weight  0.10000E+01 volume  0.46858E+03 ppm1      7.530 ppm2      0.780
ASSI [ 2754]
  (  segid "BrD " and resid 106   and name HD% )
  (( segid "BrD " and resid 106   and name HB1 ))
    2.300     1.300     1.300 peak  2754 weight  0.10000E+01 volume  0.86816E+03 ppm1      7.526 ppm2      3.919
ASSI [ 2774]
  (  segid "BrD " and resid 106   and name HD% )
  (( segid "BrD " and resid 106   and name HB2 ))
    2.400     1.400     1.400 peak  2774 weight  0.10000E+01 volume  0.63063E+03 ppm1      7.524 ppm2      3.708
ASSI [ 2834]
  (  segid "BrD " and resid 106   and name HD% )
  (  segid "BrD " and resid 107   and name HE% )
    3.400     2.900     2.100 peak  2834 weight  0.10000E+01 volume  0.82229E+02 ppm1      7.513 ppm2      7.940
ASSI [ 3074]
  (  segid "BrD " and resid 67    and name HE% )
  (  segid "BrD " and resid 73    and name HD1% )
    4.000     4.000     1.500 peak  3074 weight  0.10000E+01 volume  0.28072E+02 ppm1      7.318 ppm2      1.565
ASSI [ 3144]
  (  segid "BrD " and resid 47    and name HE% )
  (( segid "BrD " and resid 46    and name HB2 ))
    3.000     2.200     2.200 peak  3144 weight  0.10000E+01 volume  0.17782E+03 ppm1      7.270 ppm2      3.075
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ASSI ( 3224)
  (  segid "BrD " and resid 82   and name HD% )
  (( segid "BrD " and resid 103  and name HG1 ))
     3.100     2.400     2.400 peak  3224 weight  0.10000E+01 volume  0.12400E+03 ppm1     7.264 ppm2     2.595
ASSI ( 3234)
  (  segid "BrD " and resid 82   and name HD% )
  (( segid "BrD " and resid 103  and name HB1 ))
     3.200     2.600     2.300 peak  3234 weight  0.10000E+01 volume  0.10914E+03 ppm1     7.266 ppm2     2.374
ASSI ( 3254)
  (  segid "BrD " and resid 82   and name HD% )
  (( segid "BrD " and resid 81   and name HB  ))
     3.200     2.600     2.300 peak  3254 weight  0.10000E+01 volume  0.12188E+03 ppm1     7.266 ppm2     2.032
ASSI ( 3264)
  (  segid "BrD " and resid 82   and name HD% )
  (( segid "BrD " and resid 103  and name HB2 ))
     3.100     2.400     2.400 peak  3264 weight  0.10000E+01 volume  0.13715E+03 ppm1     7.266 ppm2     1.902
ASSI ( 3314)
  (  segid "BrD " and resid 82   and name HD% )
  (  segid "BrD " and resid 102  and name HD2%)
     3.100     2.400     2.400 peak  3314 weight  0.10000E+01 volume  0.13023E+03 ppm1     7.261 ppm2     1.332
OR ( 3314)
  (  segid "BrD " and resid 82   and name HD% )
  (  segid "BrD " and resid 102  and name HD1%)
ASSI ( 3354)
  (  segid "BrD " and resid 82   and name HE% )
  (( segid "BrD " and resid 106  and name HB1 ))
     3.000     2.200     2.200 peak  3354 weight  0.10000E+01 volume  0.15234E+03 ppm1     7.069 ppm2     3.922
ASSI ( 3364)
  (  segid "BrD " and resid 82   and name HE% )
  (( segid "BrD " and resid 103  and name HA  ))
     3.000     2.200     2.200 peak  3364 weight  0.10000E+01 volume  0.15998E+03 ppm1     7.070 ppm2     3.789
ASSI ( 3404)
  (  segid "BrD " and resid 82   and name HE% )
  (( segid "BrD " and resid 102  and name HB2 ))
     2.900     2.100     2.100 peak  3404 weight  0.10000E+01 volume  0.20703E+03 ppm1     7.070 ppm2     1.838
ASSI ( 3424)
  (  segid "BrD " and resid 82   and name HE% )
  (  segid "BrD " and resid 102  and name HD2%)
     2.400     1.400     1.400 peak  3424 weight  0.10000E+01 volume  0.67243E+03 ppm1     7.070 ppm2     1.333
ASSI ( 3444)
  (  segid "BrD " and resid 82   and name HE% )
  (  segid "BrD " and resid 107  and name HD% )
     3.500     3.100     2.000 peak  3444 weight  0.10000E+01 volume  0.65231E+02 ppm1     7.069 ppm2     7.777
ASSI ( 3464)
  (  segid "BrD " and resid 82   and name HE% )
  (  segid "BrD " and resid 78   and name HD2%)
     2.900     2.100     2.100 peak  3464 weight  0.10000E+01 volume  0.20065E+03 ppm1     7.067 ppm2     0.680
ASSI ( 3514)
  (( segid "BrD " and resid 82   and name HZ  ))
  (  segid "BrD " and resid 102  and name HD2%)
     3.200     2.600     2.300 peak  3514 weight  0.10000E+01 volume  0.11748E+03 ppm1     7.021 ppm2     1.331
ASSI ( 3524)
  (( segid "BrD " and resid 82   and name HZ  ))
  (  segid "BrD " and resid 78   and name HD2%)
     2.800     2.000     2.000 peak  3524 weight  0.10000E+01 volume  0.25407E+03 ppm1     7.017 ppm2     0.681
ASSI ( 3574)
  (  segid "BrD " and resid 74   and name HD% )
  (  segid "BrD " and resid 68   and name HD% )
     2.800     2.000     2.000 peak  3574 weight  0.10000E+01 volume  0.24279E+03 ppm1     7.005 ppm2     7.777
ASSI ( 3654)
  (  segid "BrD " and resid 74   and name HD% )
  (  segid "BrD " and resid 75   and name HE% )
     3.300     2.700     2.200 peak  3654 weight  0.10000E+01 volume  0.90985E+02 ppm1     7.005 ppm2     2.667
ASSI ( 3684)
  (  segid "BrD " and resid 74   and name HD% )
  (  segid "BrD " and resid 59   and name HE% )
     2.600     1.700     1.700 peak  3684 weight  0.10000E+01 volume  0.36097E+03 ppm1     7.005 ppm2     1.885
ASSI ( 3754)
  (  segid "BrD " and resid 67   and name HD% )
  (( segid "BrD " and resid 62   and name HG2 ))
     3.400     2.900     2.100 peak  3754 weight  0.10000E+01 volume  0.78199E+02 ppm1     6.899 ppm2     1.496
ASSI ( 3804)
  (  segid "BrD " and resid 46   and name HE% )
  (( segid "BrD " and resid 53   and name HA  ))
     3.100     2.400     2.400 peak  3804 weight  0.10000E+01 volume  0.13088E+03 ppm1     6.686 ppm2     4.701
ASSI ( 3944)
  (  segid "BrD " and resid 46   and name HD% )
  (  segid "BrD " and resid 38   and name HG1%)
     3.400     2.900     2.100 peak  3944 weight  0.10000E+01 volume  0.75575E+02 ppm1     5.740 ppm2     1.088
ASSI ( 4024)
  (( segid "BrD " and resid 52   and name HA  ))
  (( segid "BrD " and resid 53   and name HD2 ))
     3.400     2.900     2.100 peak  4024 weight  0.10000E+01 volume  0.78758E+02 ppm1     5.589 ppm2     4.017
ASSI ( 4054)
  (( segid "BrD " and resid 28   and name HD2 ))
  (( segid "BrD " and resid 34   and name HZ  ))
     2.800     2.000     2.000 peak  4054 weight  0.10000E+01 volume  0.24761E+03 ppm1     5.577 ppm2     7.924
ASSI ( 4114)
  (( segid "BrD " and resid 34   and name HA  ))
  (  segid "BrD " and resid 34   and name HD% )
     3.300     1.300     1.300 peak  4114 weight  0.10000E+01 volume  0.78719E+03 ppm1     5.547 ppm2     7.713
ASSI ( 4204)
  (  segid "BrD " and resid 34   and name HD% )
  (  segid "BrD " and resid 56   and name HD1%)
     2.900     2.100     2.100 peak  4204 weight  0.10000E+01 volume  0.22356E+03 ppm1     7.714 ppm2     1.544
ASSI ( 4264)
  (  segid "BrD " and resid 34   and name HE% )
  (( segid "BrD " and resid 31   and name HA  ))
     2.500     1.600     1.600 peak  4264 weight  0.10000E+01 volume  0.48557E+03 ppm1     7.781 ppm2     6.993
ASSI ( 4304)
  (  segid "BrD " and resid 107  and name HD% )
  (  segid "BrD " and resid 106  and name HD% )
     2.800     2.000     2.000 peak  4304 weight  0.10000E+01 volume  0.27783E+03 ppm1     7.802 ppm2     7.517
ASSI ( 4324)
  (( segid "BrD " and resid 82   and name HZ  ))
  (( segid "BrD " and resid 103  and name HA  ))
     3.300     2.700     2.200 peak  4324 weight  0.10000E+01 volume  0.96267E+02 ppm1     7.031 ppm2     3.790
ASSI ( 4364)
  (  segid "BrD " and resid 107  and name HE% )
  (( segid "BrD " and resid 78   and name HB2 ))
     3.400     2.900     2.100 peak  4364 weight  0.10000E+01 volume  0.78224E+02 ppm1     7.888 ppm2     1.085
ASSI (    5)
  (( segid "AcH " and resid 201  and name HA1 ))
  (  segid "BrD " and resid 38   and name HG1%)
     2.600     1.700     1.700 peak     5 weight  0.11000E+01 volume  0.16527E+03 ppm1     4.029 ppm2     1.081
OR (    5)
  (( segid "AcH " and resid 201  and name HA2 ))
  (  segid "BrD " and resid 38   and name HG1%)
ASSI (   15)
  (( segid "AcH " and resid 201  and name HA1 ))
  (  segid "BrD " and resid 38   and name HG2%)
     2.600     1.700     1.700 peak    15 weight  0.11000E+01 volume  0.14933E+03 ppm1     4.026 ppm2     0.723
OR (   15)
  (( segid "AcH " and resid 201  and name HA2 ))
  (  segid "BrD " and resid 38   and name HG2%)
ASSI (   25)
  (( segid "AcH " and resid 201  and name HA1 ))
  (  segid "BrD " and resid 43   and name HB% )
     2.600     1.700     1.700 peak    25 weight  0.11000E+01 volume  0.16374E+03 ppm1     4.023 ppm2     1.609
ASSI (   35)
  (( segid "AcH " and resid 201  and name HB2 ))
  (  segid "BrD " and resid 43   and name HB% )
     2.600     1.700     1.700 peak    35 weight  0.11000E+01 volume  0.16831E+03 ppm1     3.428 ppm2     1.601
ASSI (   45)
  (( segid "AcH " and resid 201  and name HB2 ))
  (  segid "BrD " and resid 38   and name HG1%)
     2.700     1.800     1.800 peak    45 weight  0.11000E+01 volume  0.14392E+03 ppm1     3.430 ppm2     1.074
OR (   45)
  (( segid "AcH " and resid 201  and name HB1 ))
  (  segid "BrD " and resid 38   and name HG1%)
ASSI (   55)
  (( segid "AcH " and resid 201  and name HB2 ))
  (  segid "BrD " and resid 38   and name HG2%)
     2.600     1.700     1.700 peak    55 weight  0.11000E+01 volume  0.14742E+03 ppm1     3.430 ppm2     0.723
OR (   55)
  (( segid "AcH " and resid 201  and name HB1 ))
  (  segid "BrD " and resid 38   and name HG2%)
ASSI (   65)
  (( segid "AcH " and resid 201  and name HD1 ))
  (  segid "BrD " and resid 43   and name HB% )
     2.600     1.700     1.700 peak    65 weight  0.11000E+01 volume  0.15413E+03 ppm1     8.179 ppm2     1.608
ASSI (   75)
  (( segid "AcH " and resid 201  and name HD2 ))
  (  segid "BrD " and resid 43   and name HB% )
     2.700     1.800     1.800 peak    75 weight  0.11000E+01 volume  0.13471E+03 ppm1     7.683 ppm2     1.592
ASSI (   85)
  (( segid "AcH " and resid 201  and name HD2 ))
  (  segid "BrD " and resid 38   and name HG1%)
     2.700     1.800     1.800 peak    85 weight  0.11000E+01 volume  0.12532E+03 ppm1     7.680 ppm2     1.066
ASSI (   95)
  (( segid "AcH " and resid 201  and name HD2 ))
  (  segid "BrD " and resid 38   and name HG2%)
     2.700     1.800     1.800 peak    95 weight  0.11000E+01 volume  0.12585E+03 ppm1     7.690 ppm2     0.691
ASSI (  105)
  (  segid "AcH " and resid 200  and name HA% )
  (  segid "BrD " and resid 38   and name HG2%)
     2.600     1.700     1.700 peak   105 weight  0.11000E+01 volume  0.16395E+03 ppm1     2.547 ppm2     0.727
ASSI (  115)
  (  segid "AcH " and resid 200  and name HA% )
  (  segid "BrD " and resid 38   and name HG1%)
     2.400     1.400     1.400 peak   115 weight  0.11000E+01 volume  0.29029E+03 ppm1     2.548 ppm2     1.072
ASSI (  125)
  (  segid "AcH " and resid 200  and name HA% )
  (  segid "BrD " and resid 43   and name HB% )
     2.700     1.800     1.800 peak   125 weight  0.11000E+01 volume  0.13320E+03 ppm1     2.536 ppm2     1.603
ASSI (  135)
  (  segid "AcH " and resid 200  and name HA% )
  (( segid "BrD " and resid 38   and name HA  ))
     2.600     1.700     1.700 peak   135 weight  0.11000E+01 volume  0.17326E+03 ppm1     2.548 ppm2     4.209
ASSI (  145)
  (  segid "AcH " and resid 200  and name HA% )
  (( segid "BrD " and resid 43   and name HA  ))
     2.700     1.800     1.800 peak   145 weight  0.11000E+01 volume  0.12382E+03 ppm1     2.547 ppm2     5.520
ASSI (    6)
  (( segid "AcH " and resid 201  and name HA1 ))
  (  segid "BrD " and resid 46   and name HE% )
     2.700     1.800     1.800 peak     6 weight  0.11000E+01 volume  0.14312E+03 ppm1     4.007 ppm2     6.648
OR (    6)
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   (( segid "AcH " and resid 201  and name HA2 ))
   (  segid "BrD " and resid 46   and name HE% )
 ASSI (   16)
   (( segid "AcH " and resid 201  and name HA2 ))
   (  segid "BrD " and resid 95   and name HD% )
      2.700      1.800      1.800 peak     16 weight  0.11000E+01 volume  0.13924E+03 ppm1      4.015 ppm2      7.481
 OR (   16)
   (( segid "AcH " and resid 201  and name HA1 ))
   (  segid "BrD " and resid 95   and name HD% )
 ASSI (   26)
   (( segid "AcH " and resid 201  and name HB1 ))
   (  segid "BrD " and resid 95   and name HD% )
      2.600      1.700      1.700 peak     26 weight  0.11000E+01 volume  0.15229E+03 ppm1      3.429 ppm2      7.481
 OR (   26)
   (( segid "AcH " and resid 201  and name HB2 ))
   (  segid "BrD " and resid 95   and name HD% )
 ASSI (   36)
   (( segid "AcH " and resid 201  and name HA1 ))
   (  segid "BrD " and resid 88   and name HD% )
      2.500      1.600      1.600 peak     36 weight  0.11000E+01 volume  0.18465E+03 ppm1      4.015 ppm2      7.637
 OR (   36)
   (( segid "AcH " and resid 201  and name HA2 ))
   (  segid "BrD " and resid 88   and name HD% )
 ASSI (   46)
   (( segid "AcH " and resid 201  and name HB2 ))
   (  segid "BrD " and resid 88   and name HD% )
      2.700      1.800      1.800 peak     46 weight  0.11000E+01 volume  0.13938E+03 ppm1      3.429 ppm2      7.637
 OR (   46)
   (( segid "AcH " and resid 201  and name HB1 ))
   (  segid "BrD " and resid 88   and name HD% )
 ASSI (   56)
   (( segid "AcH " and resid 201  and name HA2 ))
   (  segid "BrD " and resid 95   and name HE% )
      2.600      1.700      1.700 peak     56 weight  0.11000E+01 volume  0.16075E+03 ppm1      4.015 ppm2      7.585
 OR (   56)
   (( segid "AcH " and resid 201  and name HA1 ))
   (  segid "BrD " and resid 95   and name HE% )
 ASSI (   66)
   (( segid "AcH " and resid 201  and name HB1 ))
   (  segid "BrD " and resid 95   and name HE% )
      2.600      1.700      1.700 peak     66 weight  0.11000E+01 volume  0.16293E+03 ppm1      3.429 ppm2      7.585
 ASSI (   76)
   (  segid "AcH " and resid 200  and name HA% )
   (  segid "BrD " and resid 95   and name HE% )
      2.700      1.800      1.800 peak     76 weight  0.11000E+01 volume  0.14049E+03 ppm1      2.542 ppm2      7.585
 ASSI (   86)
   (( segid "AcH " and resid 201  and name HA1 ))
   (  segid "BrD " and resid 88   and name HE% )
      2.600      1.700      1.700 peak     86 weight  0.11000E+01 volume  0.16796E+03 ppm1      4.019 ppm2      7.358
 OR (   86)
   (( segid "AcH " and resid 201  and name HA2 ))
   (  segid "BrD " and resid 88   and name HE% )
 ASSI (   96)
   (( segid "AcH " and resid 201  and name HB2 ))
   (  segid "BrD " and resid 88   and name HE% )
      2.600      1.700      1.700 peak     96 weight  0.11000E+01 volume  0.16763E+03 ppm1      3.430 ppm2      7.358
 OR (   96)
   (( segid "AcH " and resid 201  and name HB1 ))
   (  segid "BrD " and resid 88   and name HE% )
 ASSI (    7)
   (  segid "AcH " and resid 200  and name HA% )
   (( segid "AcH " and resid 201  and name HN  ))
      2.700      1.800      1.800 peak      7 weight  0.11000E+01 volume  0.12000E+03 ppm1      3.430 ppm2      7.358
 ASSI (   17)
   (  segid "AcH " and resid 200  and name HA% )
   (( segid "AcH " and resid 201  and name HA1 ))
      2.700      1.800      1.800 peak     17 weight  0.11000E+01 volume  0.12000E+03 ppm1      3.430 ppm2      7.358
 ASSI (   27)
   (( segid "AcH " and resid 201  and name HB2 ))
   (( segid "AcH " and resid 201  and name HD1 ))
      2.700      1.800      1.800 peak     27 weight  0.11000E+01 volume  0.12000E+03 ppm1      3.430 ppm2      7.358
 OR (   27)
   (( segid "AcH " and resid 201  and name HB1 ))
   (( segid "AcH " and resid 201  and name HD1 ))
 ASSI (   37)
   (( segid "AcH " and resid 201  and name HB1 ))
   (( segid "AcH " and resid 201  and name HN  ))
      2.700      1.800      1.800 peak     37 weight  0.11000E+01 volume  0.12000E+03 ppm1      3.430 ppm2      7.358
 OR (   37)
   (( segid "AcH " and resid 201  and name HB2 ))
   (( segid "AcH " and resid 201  and name HN  ))
 ASSI (   47)
   (( segid "AcH " and resid 201  and name HA2 ))
   (( segid "AcH " and resid 201  and name HN  ))
      2.700      1.800      1.800 peak     47 weight  0.11000E+01 volume  0.12000E+03 ppm1      3.430 ppm2      7.358
 OR (   47)
   (( segid "AcH " and resid 201  and name HA1 ))
   (( segid "AcH " and resid 201  and name HN  ))
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Table 3

Ambiguous NOE-derived Inter-proton Distance Restraints

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ASSI ( 311)
  (( segid "BrD " and resid 32   and name HN  ))
  (( segid "BrD " and resid 35   and name HG1 ))
    4.200     4.200     1.300 peak   311 weight  0.10000E+01 volume  0.35526E+02 ppm1      7.738 ppm2      3.430
OR ( 311)
  (( segid "BrD " and resid 32   and name HN  ))
  (( segid "BrD " and resid 28   and name HB2 ))
ASSI ( 391)
  (( segid "BrD " and resid 106  and name HN  ))
  ( segid "BrD " and resid 105  and name HD% )
    3.100     2.400     2.400 peak   391 weight  0.10000E+01 volume  0.20417E+03 ppm1      9.740 ppm2      7.778
OR ( 391)
  (( segid "BrD " and resid 106  and name HN  ))
  (( segid "BrD " and resid 104  and name HN  ))
OR ( 391)
  (( segid "BrD " and resid 106  and name HN  ))
  ( segid "BrD " and resid 107  and name HD% )
ASSI ( 731)
  (( segid "BrD " and resid 100  and name HN  ))
  (( segid "BrD " and resid 97   and name HA  ))
    3.300     2.700     2.200 peak   731 weight  0.10000E+01 volume  0.15089E+03 ppm1      8.669 ppm2      4.801
OR ( 731)
  (( segid "BrD " and resid 100  and name HN  ))
  (( segid "BrD " and resid 98   and name HA  ))
ASSI ( 781)
  (( segid "BrD " and resid 97   and name HN  ))
  (( segid "BrD " and resid 98   and name HB2 ))
    4.000     4.000     1.500 peak   781 weight  0.10000E+01 volume  0.45845E+02 ppm1      8.671 ppm2      3.671
OR ( 781)
  (( segid "BrD " and resid 97   and name HN  ))
  (( segid "BrD " and resid 65   and name HB2 ))
ASSI ( 831)
  (( segid "BrD " and resid 96   and name HN  ))
  (( segid "BrD " and resid 97   and name HB1 ))
    3.200     2.600     2.300 peak   831 weight  0.10000E+01 volume  0.17645E+03 ppm1      7.977 ppm2      2.728
OR ( 831)
  (( segid "BrD " and resid 78   and name HN  ))
  (( segid "BrD " and resid 79   and name HB2 ))
OR ( 831)
  (( segid "BrD " and resid 77   and name HN  ))
  (( segid "BrD " and resid 79   and name HB2 ))
OR ( 831)
  (( segid "BrD " and resid 96   and name HN  ))
  (( segid "BrD " and resid 92   and name HB1 ))
OR ( 831)
  (( segid "BrD " and resid 78   and name HN  ))
  (( segid "BrD " and resid 79   and name HB1 ))
ASSI ( 1051)
  (( segid "BrD " and resid 76   and name HN  ))
  (( segid "BrD " and resid 73   and name HB2 ))
    5.000     5.000     0.500 peak  1051 weight  0.10000E+01 volume  0.12021E+02 ppm1      8.612 ppm2      2.497
OR ( 1051)
  (( segid "BrD " and resid 76   and name HN  ))
  (( segid "BrD " and resid 80   and name HB2 ))
ASSI ( 1101)
  (( segid "BrD " and resid 75   and name HN  ))
  (( segid "BrD " and resid 18   and name HG  ))
    5.500     5.500     0.000 peak  1101 weight  0.10000E+01 volume  0.63178E+01 ppm1      9.107 ppm2      2.294
OR ( 1101)
  (( segid "BrD " and resid 75   and name HN  ))
  (( segid "BrD " and resid 72   and name HD1 ))
OR ( 1101)
  (( segid "BrD " and resid 98   and name HN  ))
  ( segid "BrD " and resid 31   and name HB% )
ASSI ( 1551)
  (( segid "BrD " and resid 21   and name HN  ))
  (( segid "BrD " and resid 24   and name HE22))
    3.400     2.900     2.100 peak  1551 weight  0.10000E+01 volume  0.12608E+03 ppm1      8.544 ppm2      7.515
OR ( 1551)
  (( segid "BrD " and resid 21   and name HN  ))
  ( segid "BrD " and resid 106  and name HD% )
OR ( 1551)
  (( segid "BrD " and resid 109  and name HN  ))
  ( segid "BrD " and resid 106  and name HD% )
OR ( 1551)
  (( segid "BrD " and resid 64   and name HN  ))
  ( segid "BrD " and resid 15   and name HE% )
ASSI ( 1781)
  (( segid "BrD " and resid 26   and name HN  ))
  (( segid "BrD " and resid 22   and name HB1 ))
    3.400     2.900     2.100 peak  1781 weight  0.10000E+01 volume  0.12549E+03 ppm1      9.196 ppm2      2.672
OR ( 1781)
  (( segid "BrD " and resid 26   and name HN  ))
  (( segid "BrD " and resid 56   and name HB1 ))
ASSI ( 2721)
  (( segid "BrD " and resid 106  and name HN  ))
  (( segid "BrD " and resid 105  and name HB2 ))
    3.300     2.700     2.200 peak  2721 weight  0.10000E+01 volume  0.14753E+03 ppm1      7.763 ppm2      3.671
OR ( 2721)
  (( segid "BrD " and resid 106  and name HN  ))
  (( segid "BrD " and resid 107  and name HB1 ))
OR ( 2721)
  (( segid "BrD " and resid 106  and name HN  ))
  (( segid "BrD " and resid 106  and name HB2 ))
ASSI ( 3261)
  (( segid "BrD " and resid 16   and name HN  ))
  (( segid "BrD " and resid 13   and name HG2 ))
    4.100     4.100     1.400 peak  3261 weight  0.10000E+01 volume  0.41938E+02 ppm1      8.794 ppm2      2.954
OR ( 3261)
  (( segid "BrD " and resid 16   and name HN  ))
  (( segid "BrD " and resid 11   and name HB1 ))
ASSI ( 3361)
  (( segid "BrD " and resid 13   and name HN  ))
  (( segid "BrD " and resid 13   and name HG1 ))
    4.100     4.100     1.400 peak  3361 weight  0.10000E+01 volume  0.40202E+02 ppm1      8.809 ppm2      3.103
OR ( 3361)
  (( segid "BrD " and resid 14   and name HN  ))
  (( segid "BrD " and resid 13   and name HG1 ))
ASSI ( 3371)
  (( segid "BrD " and resid 13   and name HN  ))
  (( segid "BrD " and resid 13   and name HG2 ))
    3.300     2.700     2.200 peak  3371 weight  0.10000E+01 volume  0.14859E+03 ppm1      8.802 ppm2      2.987
OR ( 3371)
  (( segid "BrD " and resid 14   and name HN  ))
  (( segid "BrD " and resid 13   and name HG2 ))
ASSI ( 3401)
  (( segid "BrD " and resid 13   and name HN  ))
  (( segid "BrD " and resid 11   and name HD1 ))
    3.800     3.600     1.700 peak  3401 weight  0.10000E+01 volume  0.67241E+02 ppm1      8.810 ppm2      4.488
OR ( 3401)
  (( segid "BrD " and resid 14   and name HN  ))
  (( segid "BrD " and resid 11   and name HD1 ))
OR ( 3401)
  (( segid "BrD " and resid 14   and name HN  ))
  (( segid "BrD " and resid 16   and name HA  ))
ASSI ( 3671)
  (( segid "BrD " and resid 102  and name HN  ))
  (( segid "BrD " and resid 30   and name HB1 ))
    3.800     3.600     1.700 peak  3671 weight  0.10000E+01 volume  0.58619E+02 ppm1      9.156 ppm2      4.934
OR ( 3671)
  (( segid "BrD " and resid 102  and name HN  ))
  (( segid "BrD " and resid 100  and name HA  ))
ASSI ( 3841)
  (( segid "BrD " and resid 103  and name HN  ))
  (( segid "BrD " and resid 100  and name HA  ))
    3.000     2.200     2.200 peak  3841 weight  0.10000E+01 volume  0.24821E+03 ppm1      8.661 ppm2      4.900
OR ( 3841)
  (( segid "BrD " and resid 40   and name HN  ))
  (( segid "BrD " and resid 41   and name HB  ))
ASSI ( 3911)
  (( segid "BrD " and resid 59   and name HN  ))
  (( segid "BrD " and resid 57   and name HB1 ))
    3.500     3.100     2.000 peak  3911 weight  0.10000E+01 volume  0.98690E+02 ppm1      8.496 ppm2      2.969
OR ( 3911)
  (( segid "BrD " and resid 59   and name HN  ))
  (( segid "BrD " and resid 61   and name HG1 ))
OR ( 3911)
  (( segid "BrD " and resid 31   and name HN  ))
  (( segid "BrD " and resid 29   and name HG1 ))
OR ( 3911)
  (( segid "BrD " and resid 59   and name HN  ))
  (( segid "BrD " and resid 55   and name HB1 ))
ASSI ( 4131)
  (( segid "BrD " and resid 25   and name HN  ))
  (( segid "BrD " and resid 21   and name HB  ))
    3.800     3.600     1.700 peak  4131 weight  0.10000E+01 volume  0.59139E+02 ppm1      9.133 ppm2      2.465
OR ( 4131)
  (( segid "BrD " and resid 25   and name HN  ))
  (( segid "BrD " and resid 26   and name HB1 ))
ASSI ( 6751)
  (( segid "BrD " and resid 111  and name HN  ))
  (( segid "BrD " and resid 111  and name HD1 ))
    3.200     2.600     2.300 peak  6751 weight  0.10000E+01 volume  0.16212E+03 ppm1      8.168 ppm2      2.204
OR ( 6751)
  (( segid "BrD " and resid 111  and name HN  ))
  (( segid "BrD " and resid 109  and name HB2 ))
ASSI ( 6861)
  (( segid "BrD " and resid 21   and name HN  ))
  (( segid "BrD " and resid 24   and name HG2 ))
    3.400     2.900     2.100 peak  6861 weight  0.10000E+01 volume  0.12194E+03 ppm1      8.574 ppm2      3.072
OR ( 6861)
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   (( segid "BrD " and resid 21   and name HN  ))
   (( segid "BrD " and resid 24   and name HB2 ))
OR [ 6861]
   (( segid "BrD " and resid 21   and name HN  ))
   (( segid "BrD " and resid 23   and name HG2 ))
OR [ 6861]
   (( segid "BrD " and resid 21   and name HN  ))
   (( segid "BrD " and resid 24   and name HB1 ))
ASSI [ 6871]
   (( segid "BrD " and resid 21   and name HN  ))
   (( segid "BrD " and resid 22   and name HB1 ))
     3.300      2.700      2.200 peak  6871 weight  0.10000E+01 volume  0.15992E+03 ppm1      8.573 ppm2      2.702
OR [ 6871]
   (( segid "BrD " and resid 64   and name HN  ))
   (( segid "BrD " and resid 61   and name HB2 ))
OR [ 6871]
   (( segid "BrD " and resid 109  and name HN  ))
   (( segid "BrD " and resid 112  and name HB1 ))
OR [ 6871]
   (( segid "BrD " and resid 64   and name HN  ))
   (( segid "BrD " and resid 22   and name HB1 ))
ASSI [ 6911]
   (( segid "BrD " and resid 86   and name HN  ))
   (( segid "BrD " and resid 86   and name HE1 ))
     3.700      3.400      1.800 peak  6911 weight  0.10000E+01 volume  0.78171E+02 ppm1      8.423 ppm2      3.044
OR [ 6911]
   (( segid "BrD " and resid 86   and name HN  ))
   (( segid "BrD " and resid 87   and name HG1 ))
ASSI [ 7031]
   (( segid "BrD " and resid 52   and name HN  ))
   (( segid "BrD " and resid 80   and name HN  ))
     4.200      4.200      1.300 peak  7031 weight  0.10000E+01 volume  0.35356E+02 ppm1      9.003 ppm2      7.979
OR [ 7031]
   (( segid "BrD " and resid 52   and name HN  ))
   (( segid "BrD " and resid 77   and name HN  ))
OR [ 7031]
   (( segid "BrD " and resid 52   and name HN  ))
   ( segid "BrD " and resid 47   and name HD% )
ASSI [ 7121]
   (( segid "BrD " and resid 89   and name HD21))
   (( segid "BrD " and resid 85   and name HA  ))
     3.700      3.400      1.800 peak  7121 weight  0.10000E+01 volume  0.76700E+02 ppm1      8.923 ppm2      5.021
OR [ 7121]
   (( segid "BrD " and resid 89   and name HD21))
   (( segid "BrD " and resid 93   and name HB1 ))
ASSI [ 7131]
   (( segid "BrD " and resid 89   and name HD22))
   (( segid "BrD " and resid 85   and name HA  ))
     3.600      3.200      1.900 peak  7131 weight  0.10000E+01 volume  0.84076E+02 ppm1      8.416 ppm2      5.021
OR [ 7131]
   (( segid "BrD " and resid 89   and name HD22))
   (( segid "BrD " and resid 93   and name HB1 ))
ASSI [ 7251]
   (( segid "BrD " and resid 26   and name HN  ))
   ( segid "BrD " and resid 22   and name HD2% )
     3.000      2.200      2.200 peak  7251 weight  0.10000E+01 volume  0.24489E+03 ppm1      9.196 ppm2      1.549
OR [ 7251]
   (( segid "BrD " and resid 26   and name HN  ))
   ( segid "BrD " and resid 56   and name HD1% )
ASSI [ 8181]
   (( segid "BrD " and resid 57   and name HN  ))
   ( segid "BrD " and resid 25   and name HG2% )
     4.100      4.100      1.400 peak  8181 weight  0.10000E+01 volume  0.42960E+03 ppm1      9.359 ppm2      1.667
OR [ 8181]
   (( segid "BrD " and resid 57   and name HN  ))
   ( segid "BrD " and resid 58   and name HG2% )
OR [ 8181]
   (( segid "BrD " and resid 57   and name HN  ))
   ( segid "BrD " and resid 22   and name HD1% )
ASSI [ 8211]
   (( segid "BrD " and resid 114  and name HN  ))
   (( segid "BrD " and resid 111  and name HB2 ))
     4.000      4.000      1.500 peak  8211 weight  0.10000E+01 volume  0.47918E+02 ppm1      8.377 ppm2      2.377
OR [ 8211]
   (( segid "BrD " and resid 114  and name HN  ))
   (( segid "BrD " and resid 110  and name HB  ))
ASSI [ 8261]
   (( segid "BrD " and resid 28   and name HN  ))
   (( segid "BrD " and resid 25   and name HB  ))
     4.200      4.200      1.300 peak  8261 weight  0.10000E+01 volume  0.36987E+02 ppm1      8.166 ppm2      3.014
OR [ 8261]
   (( segid "BrD " and resid 28   and name HN  ))
   (( segid "BrD " and resid 29   and name HG1 ))
ASSI [ 8291]
   (( segid "BrD " and resid 28   and name HN  ))
   ( segid "BrD " and resid 25   and name HG2% )
     4.400      4.400      1.100 peak  8291 weight  0.10000E+01 volume  0.24897E+03 ppm1      8.164 ppm2      1.639
OR [ 8291]
   (( segid "BrD " and resid 28   and name HN  ))
   (( segid "BrD " and resid 26   and name HG1 ))
ASSI [ 8381]
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   (( segid "BrD " and resid 61   and name HN  ))
   ( segid "BrD " and resid 58   and name HG2% )
     3.400      2.900      2.100 peak  8381 weight  0.10000E+01 volume  0.13119E+03 ppm1      8.743 ppm2      1.674
OR [ 8381]
   (( segid "BrD " and resid 61   and name HN  ))
   ( segid "BrD " and resid 22   and name HD1% )
OR [ 8381]
   (( segid "BrD " and resid 38   and name HN  ))
   ( segid "BrD " and resid 43   and name HB% )
ASSI [ 8391]
   (( segid "BrD " and resid 38   and name HN  ))
   (( segid "BrD " and resid 39   and name HG1 ))
     4.000      4.000      1.500 peak  8391 weight  0.10000E+01 volume  0.45211E+02 ppm1      8.743 ppm2      2.008
OR [ 8391]
   (( segid "BrD " and resid 61   and name HN  ))
   (( segid "BrD " and resid 57   and name HG2 ))
ASSI [ 8511]
   (( segid "BrD " and resid 50   and name HN  ))
   (( segid "BrD " and resid 53   and name HG1 ))
     3.700      3.400      1.800 peak  8511 weight  0.10000E+01 volume  0.70210E+02 ppm1      8.564 ppm2      2.814
OR [ 8511]
   (( segid "BrD " and resid 50   and name HN  ))
   (( segid "BrD " and resid 53   and name HB1 ))
OR [ 8511]
   (( segid "BrD " and resid 50   and name HN  ))
   (( segid "BrD " and resid 87   and name HB1 ))
OR [ 8511]
   (( segid "BrD " and resid 46   and name HN  ))
   (( segid "BrD " and resid 83   and name HG1 ))
OR [ 8511]
   (( segid "BrD " and resid 46   and name HN  ))
   (( segid "BrD " and resid 53   and name HB1 ))
ASSI [ 8751]
   (( segid "BrD " and resid 58   and name HN  ))
   (( segid "BrD " and resid 37   and name HG1 ))
     3.400      2.900      2.100 peak  8751 weight  0.10000E+01 volume  0.12911E+03 ppm1     10.051 ppm2      2.747
OR [ 8751]
   (( segid "BrD " and resid 58   and name HN  ))
   ( segid "BrD " and resid 35   and name HE% )
ASSI [ 8861]
   (( segid "BrD " and resid 9    and name HN  ))
   (( segid "BrD " and resid 6    and name HG1 ))
     3.600      3.200      1.900 peak  8861 weight  0.10000E+01 volume  0.86153E+02 ppm1      9.052 ppm2      2.631
OR [ 8861]
   (( segid "BrD " and resid 9    and name HN  ))
   (( segid "BrD " and resid 7    and name HB1 ))
ASSI [ 8891]
   (( segid "BrD " and resid 103  and name HN  ))
   (( segid "BrD " and resid 100  and name HA  ))
     4.000      4.000      1.500 peak  8891 weight  0.10000E+01 volume  0.44524E+02 ppm1      8.668 ppm2      4.917
OR [ 8891]
   (( segid "BrD " and resid 112  and name HN  ))
   (( segid "BrD " and resid 113  and name HA  ))
ASSI [ 8901]
   (( segid "BrD " and resid 112  and name HN  ))
   (( segid "BrD " and resid 108  and name HA  ))
     3.400      2.900      2.100 peak  8901 weight  0.10000E+01 volume  0.11279E+03 ppm1      8.668 ppm2      4.805
OR [ 8901]
   (( segid "BrD " and resid 103  and name HN  ))
   (( segid "BrD " and resid 82   and name HA  ))
OR [ 8901]
   (( segid "BrD " and resid 103  and name HN  ))
   (( segid "BrD " and resid 98   and name HA  ))
ASSI [ 8911]
   (( segid "BrD " and resid 103  and name HN  ))
   (( segid "BrD " and resid 99   and name HA  ))
     3.500      3.100      2.000 peak  8911 weight  0.10000E+01 volume  0.10762E+03 ppm1      8.668 ppm2      4.426
OR [ 8911]
   (( segid "BrD " and resid 112  and name HN  ))
   (( segid "BrD " and resid 110  and name HA  ))
ASSI [ 8941]
   (( segid "BrD " and resid 103  and name HN  ))
   ( segid "BrD " and resid 99   and name HB% )
     2.900      2.100      3.100 peak  8941 weight  0.10000E+01 volume  0.39817E+03 ppm1      8.667 ppm2      2.178
OR [ 8941]
   (( segid "BrD " and resid 103  and name HN  ))
   (( segid "BrD " and resid 102  and name HG  ))
OR [ 8941]
   (( segid "BrD " and resid 112  and name HN  ))
   (( segid "BrD " and resid 109  and name HB2 ))
ASSI [ 9011]
   (( segid "BrD " and resid 105  and name HN  ))
   (( segid "BrD " and resid 104  and name HD1 ))
     3.100      2.400      2.400 peak  9011 weight  0.10000E+01 volume  0.22428E+03 ppm1      8.487 ppm2      2.294
OR [ 9011]
   (( segid "BrD " and resid 105  and name HN  ))
   (( segid "BrD " and resid 103  and name HB1 ))
ASSI [ 9031]
   (( segid "BrD " and resid 105  and name HN  ))
   (( segid "BrD " and resid 102  and name HB2 ))
     3.800      3.600      1.700 peak  9031 weight  0.10000E+01 volume  0.62331E+02 ppm1      8.487 ppm2      1.805
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OR ( 9011)
  (( segid "BrD " and resid 105  and name HN  ))
  (  segid "BrD " and resid 25   and name HG1%)
ASSI ( 9091)
  (( segid "BrD " and resid 109  and name HN  ))
  (( segid "BrD " and resid 106  and name HB2 ))
    3.400      3.600      1.700 peak  9091 weight  0.10000E+01 volume  0.66318E+02 ppm1      8.574 ppm2      3.678
OR ( 9091)
  (( segid "BrD " and resid 109  and name HN  ))
  (( segid "BrD " and resid 107  and name HB1 ))
OR ( 9091)
  (( segid "BrD " and resid 109  and name HN  ))
  (( segid "BrD " and resid 105  and name HB2 ))
OR ( 9091)
  (( segid "BrD " and resid 64   and name HN  ))
  (( segid "BrD " and resid 68   and name HB1 ))
ASSI ( 9101)
  (( segid "BrD " and resid 64   and name HN  ))
  (( segid "BrD " and resid 63   and name HB2 ))
    2.900      2.100      2.100 peak  9101 weight  0.10000E+01 volume  0.30416E+03 ppm1      8.573 ppm2      2.498
OR ( 9101)
  (( segid "BrD " and resid 21   and name HN  ))
  (( segid "BrD " and resid 21   and name HB  ))
ASSI ( 9111)
  (( segid "BrD " and resid 21   and name HN  ))
  (  segid "BrD " and resid 17   and name HG2%)
    3.500      3.100      2.000 peak  9111 weight  0.10000E+01 volume  0.10029E+03 ppm1      8.574 ppm2      1.725
OR ( 9111)
  (( segid "BrD " and resid 109  and name HN  ))
  (  segid "BrD " and resid 17   and name HG2%)
ASSI ( 9161)
  (( segid "BrD " and resid 106  and name HN  ))
  (( segid "BrD " and resid 104  and name HB1 ))
    3.900      3.800      1.600 peak  9161 weight  0.10000E+01 volume  0.56197E+02 ppm1      9.740 ppm2      2.560
OR ( 9161)
  (( segid "BrD " and resid 106  and name HN  ))
  (( segid "BrD " and resid 103  and name HG2 ))
ASSI ( 9171)
  (( segid "BrD " and resid 106  and name HN  ))
  (( segid "BrD " and resid 109  and name HB1 ))
    4.000      4.000      1.500 peak  9171 weight  0.10000E+01 volume  0.47295E+02 ppm1      9.739 ppm2      2.318
OR ( 9171)
  (( segid "BrD " and resid 106  and name HN  ))
  (( segid "BrD " and resid 103  and name HB1 ))
OR ( 9171)
  (( segid "BrD " and resid 106  and name HN  ))
  (( segid "BrD " and resid 104  and name HD1 ))
OR ( 9171)
  (( segid "BrD " and resid 106  and name HN  ))
  (( segid "BrD " and resid 21   and name HG11))
ASSI ( 9181)
  (( segid "BrD " and resid 106  and name HN  ))
  (( segid "BrD " and resid 102  and name HG  ))
    4.100      4.100      1.400 peak  9181 weight  0.10000E+01 volume  0.40041E+02 ppm1      9.742 ppm2      2.150
OR ( 9181)
  (( segid "BrD " and resid 106  and name HN  ))
  (( segid "BrD " and resid 109  and name HB2 ))
ASSI ( 9191)
  (( segid "BrD " and resid 106  and name HN  ))
  (( segid "BrD " and resid 102  and name HB1 ))
    4.200      4.200      1.300 peak  9191 weight  0.10000E+01 volume  0.35794E+02 ppm1      9.740 ppm2      2.002
OR ( 9191)
  (( segid "BrD " and resid 106  and name HN  ))
  (( segid "BrD " and resid 109  and name HD1 ))
ASSI ( 9201)
  (( segid "BrD " and resid 106  and name HN  ))
  (( segid "BrD " and resid 102  and name HB2 ))
    3.900      3.800      1.600 peak  9201 weight  0.10000E+01 volume  0.56482E+02 ppm1      9.739 ppm2      1.786
OR ( 9201)
  (( segid "BrD " and resid 106  and name HN  ))
  (  segid "BrD " and resid 25   and name HG1%)
ASSI ( 9241)
  (( segid "BrD " and resid 84   and name HN  ))
  (( segid "BrD " and resid 80   and name HD2 ))
    3.700      3.400      1.800 peak  9241 weight  0.10000E+01 volume  0.69670E+02 ppm1      9.464 ppm2      3.908
OR ( 9241)
  (( segid "BrD " and resid 84   and name HN  ))
  (( segid "BrD " and resid 85   and name HB1 ))
ASSI ( 9251)
  (( segid "BrD " and resid 63   and name HN  ))
  (( segid "BrD " and resid 62   and name HG1 ))
    3.700      3.400      1.800 peak  9251 weight  0.10000E+01 volume  0.78060E+02 ppm1      9.463 ppm2      2.352
OR ( 9251)
  (( segid "BrD " and resid 84   and name HN  ))
  (( segid "BrD " and resid 80   and name HG1 ))
OR ( 9251)
  (( segid "BrD " and resid 84   and name HN  ))
  (( segid "BrD " and resid 86   and name HB1 ))
ASSI ( 9281)
  (( segid "BrD " and resid 84   and name HN  ))
  (( segid "BrD " and resid 80   and name HN  ))
    3.300      2.700      2.200 peak  9281 weight  0.10000E+01 volume  0.13642E+03 ppm1      9.462 ppm2      6.001
OR ( 9281)
  (( segid "BrD " and resid 84   and name HN  ))
  (( segid "BrD " and resid 107  and name HZ  ))
OR ( 9281)
  (( segid "BrD " and resid 63   and name HN  ))
  (( segid "BrD " and resid 70   and name HN  ))
ASSI ( 9311)
  (( segid "BrD " and resid 22   and name HN  ))
  (( segid "BrD " and resid 22   and name HA  ))
    4.200      4.200      1.300 peak  9311 weight  0.10000E+01 volume  0.35671E+02 ppm1      9.473 ppm2      4.678
OR ( 9311)
  (( segid "BrD " and resid 84   and name HN  ))
  (( segid "BrD " and resid 80   and name HA  ))
ASSI ( 9341)
  (( segid "BrD " and resid 63   and name HN  ))
  (  segid "BrD " and resid 74   and name HE% )
    2.900      2.100      2.100 peak  9341 weight  0.10000E+01 volume  0.30219E+03 ppm1      9.456 ppm2      7.510
OR ( 9341)
  (( segid "BrD " and resid 22   and name HN  ))
  (  segid "BrD " and resid 106  and name HD% )
ASSI ( 9371)
  (( segid "BrD " and resid 22   and name HN  ))
  (( segid "BrD " and resid 24   and name HG2 ))
    3.400      2.900      2.100 peak  9371 weight  0.10000E+01 volume  0.12105E+03 ppm1      9.456 ppm2      3.066
OR ( 9371)
  (( segid "BrD " and resid 22   and name HN  ))
  (( segid "BrD " and resid 23   and name HG2 ))
OR ( 9371)
  (( segid "BrD " and resid 63   and name HN  ))
  (( segid "BrD " and resid 59   and name HG2 ))
ASSI ( 9441)
  (( segid "BrD " and resid 109  and name HN  ))
  (( segid "BrD " and resid 109  and name HB2 ))
    3.900      3.800      1.600 peak  9441 weight  0.10000E+01 volume  0.55505E+02 ppm1      8.557 ppm2      2.173
OR ( 9441)
  (( segid "BrD " and resid 64   and name HN  ))
  (( segid "BrD " and resid 64   and name HG1 ))
ASSI ( 9451)
  (( segid "BrD " and resid 21   and name HN  ))
  (( segid "BrD " and resid 24   and name HG2 ))
    3.900      3.800      1.600 peak  9451 weight  0.10000E+01 volume  0.53501E+02 ppm1      8.556 ppm2      3.108
OR ( 9451)
  (( segid "BrD " and resid 21   and name HN  ))
  (( segid "BrD " and resid 24   and name HB2 ))
OR ( 9451)
  (( segid "BrD " and resid 21   and name HN  ))
  (( segid "BrD " and resid 23   and name HG1 ))
OR ( 9451)
  (( segid "BrD " and resid 21   and name HN  ))
  (( segid "BrD " and resid 24   and name HB1 ))
ASSI ( 9461)
  (( segid "BrD " and resid 64   and name HN  ))
  (( segid "BrD " and resid 61   and name HB1 ))
    3.700      3.400      1.800 peak  9461 weight  0.10000E+01 volume  0.72347E+02 ppm1      8.544 ppm2      2.851
OR ( 9461)
  (( segid "BrD " and resid 21   and name HN  ))
  (( segid "BrD " and resid 23   and name HB2 ))
ASSI ( 9491)
  (( segid "BrD " and resid 21   and name HN  ))
  (( segid "BrD " and resid 19   and name HB2 ))
    3.300      2.700      2.200 peak  9491 weight  0.10000E+01 volume  0.14127E+03 ppm1      8.556 ppm2      1.929
OR ( 9491)
  (( segid "BrD " and resid 109  and name HN  ))
  (( segid "BrD " and resid 111  and name HG2 ))
OR ( 9491)
  (( segid "BrD " and resid 109  and name HN  ))
  (  segid "BrD " and resid 113  and name HB% )
OR ( 9491)
  (( segid "BrD " and resid 64   and name HN  ))
  (( segid "BrD " and resid 19   and name HB2 ))
ASSI ( 9501)
  (( segid "BrD " and resid 21   and name HN  ))
  (  segid "BrD " and resid 17   and name HG2%)
    3.300      2.700      2.200 peak  9501 weight  0.10000E+01 volume  0.14396E+03 ppm1      8.556 ppm2      1.762
OR ( 9501)
  (( segid "BrD " and resid 109  and name HN  ))
  (  segid "BrD " and resid 17   and name HG2%)
OR ( 9501)
  (( segid "BrD " and resid 21   and name HN  ))
  (  segid "BrD " and resid 25   and name HG1%)
ASSI ( 9531)
  (( segid "BrD " and resid 17   and name HN  ))
  (( segid "BrD " and resid 13   and name HA  ))
    3.600      3.200      1.900 peak  9531 weight  0.10000E+01 volume  0.86367E+02 ppm1      8.695 ppm2      4.805
OR ( 9531)
  (( segid "BrD " and resid 113  and name HN  ))
  (( segid "BrD " and resid 108  and name HA  ))
OR ( 9531)
  (( segid "BrD " and resid 103  and name HN  ))
  (( segid "BrD " and resid 82   and name HA  ))
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ASSI ( 9561)
  (( segid "BrD " and resid 103  and name HN  ))
  (( segid "BrD " and resid 106  and name HB2 ))
     3.300      2.700      2.200 peak  9561 weight  0.10000E+01 volume  0.15504E+03 ppm1       8.696 ppm2       3.661
OR ( 9561)
  (( segid "BrD " and resid 103  and name HN  ))
  (( segid "BrD " and resid 82   and name HB1 ))
OR ( 9561)
  (( segid "BrD " and resid 103  and name HN  ))
  (( segid "BrD " and resid 105  and name HB2 ))
OR ( 9561)
  (( segid "BrD " and resid 103  and name HN  ))
  (( segid "BrD " and resid 107  and name HB1 ))
ASSI ( 9631)
  (( segid "BrD " and resid 99   and name HN  ))
  (( segid "BrD " and resid 100  and name HA  ))
     3.900      3.800      1.600 peak  9631 weight  0.10000E+01 volume  0.54041E+02 ppm1       8.936 ppm2       4.947
OR ( 9631)
  (( segid "BrD " and resid 99   and name HN  ))
  (( segid "BrD " and resid 30   and name HB1 ))
ASSI ( 9641)
  (( segid "BrD " and resid 99   and name HN  ))
  (( segid "BrD " and resid 101  and name HG11))
     3.900      3.800      1.600 peak  9641 weight  0.10000E+01 volume  0.56248E+02 ppm1       8.935 ppm2       2.460
OR ( 9641)
  (( segid "BrD " and resid 99   and name HN  ))
  (( segid "BrD " and resid 97   and name HG1 ))
ASSI ( 9651)
  (( segid "BrD " and resid 99   and name HN  ))
  (( segid "BrD " and resid 103  and name HB2 ))
     5.500      5.500      0.000 peak  9651 weight  0.10000E+01 volume  0.57216E-02 ppm1       8.936 ppm2       1.920
OR ( 9651)
  (( segid "BrD " and resid 99   and name HN  ))
  (( segid "BrD " and resid 86   and name HG1 ))
ASSI ( 9721)
  (( segid "BrD " and resid 64   and name HN  ))
  (( segid "BrD " and resid 64   and name HE1 ))
     4.000      4.000      1.500 peak  9721 weight  0.10000E+01 volume  0.46621E+02 ppm1       8.586 ppm2       3.626
OR ( 9721)
  (( segid "BrD " and resid 64   and name HN  ))
  (( segid "BrD " and resid 65   and name HB1 ))
ASSI ( 9731)
  (( segid "BrD " and resid 21   and name HN  ))
  (( segid "BrD " and resid 109  and name HE1 ))
     3.800      3.600      1.700 peak  9731 weight  0.10000E+01 volume  0.59335E+02 ppm1       8.584 ppm2       3.146
OR ( 9731)
  (( segid "BrD " and resid 21   and name HN  ))
  (( segid "BrD " and resid 23   and name HG1 ))
ASSI ( 9801)
  (( segid "BrD " and resid 103  and name HN  ))
  (( segid "BrD " and resid 106  and name HB2 ))
     4.600      4.600      0.900 peak  9801 weight  0.10000E+01 volume  0.19838E+02 ppm1       8.669 ppm2       3.659
OR ( 9801)
  (( segid "BrD " and resid 17   and name HN  ))
  (( segid "BrD " and resid 15   and name HB2 ))
OR ( 9801)
  (( segid "BrD " and resid 103  and name HN  ))
  (( segid "BrD " and resid 82   and name HB1 ))
OR ( 9801)
  (( segid "BrD " and resid 103  and name HN  ))
  (( segid "BrD " and resid 105  and name HB2 ))
ASSI ( 9821)
  (( segid "BrD " and resid 17   and name HN  ))
  (( segid "BrD " and resid 13   and name HG2 ))
     3.700      3.400      1.800 peak  9821 weight  0.10000E+01 volume  0.70791E+02 ppm1       8.668 ppm2       2.943
OR ( 9821)
  (( segid "BrD " and resid 17   and name HN  ))
  (( segid "BrD " and resid 11   and name HB1 ))
ASSI ( 9831)
  (( segid "BrD " and resid 17   and name HN  ))
  (( segid "BrD " and resid 18   and name HG  ))
     3.000      2.200      2.200 peak  9831 weight  0.10000E+01 volume  0.24267E+03 ppm1       8.669 ppm2       2.284
OR ( 9831)
  (( segid "BrD " and resid 40   and name HN  ))
  (( segid "BrD " and resid 39   and name HD1 ))
OR ( 9831)
  (( segid "BrD " and resid 103  and name HN  ))
  (( segid "BrD " and resid 104  and name HD1 ))
ASSI ( 9841)
  (( segid "BrD " and resid 103  and name HN  ))
  (( segid "BrD " and resid 102  and name HB1 ))
     4.500      4.500      1.000 peak  9841 weight  0.10000E+01 volume  0.24619E+02 ppm1       8.669 ppm2       1.973
OR ( 9841)
  (( segid "BrD " and resid 17   and name HN  ))
  (  segid "BrD " and resid 113  and name HB% )
ASSI ( 9861)
  (( segid "BrD " and resid 17   and name HN  ))
  (( segid "BrD " and resid 14   and name HB2 ))
     3.500      3.100      2.000 peak  9861 weight  0.10000E+01 volume  0.99899E+02 ppm1       8.668 ppm2       2.135
OR ( 9861)
  (( segid "BrD " and resid 17   and name HN  ))
  (( segid "BrD " and resid 18   and name HB1 ))
OR ( 9861)
  (( segid "BrD " and resid 103  and name HN  ))
  (( segid "BrD " and resid 104  and name HG1 ))
ASSI (10081)
  (( segid "BrD " and resid 24   and name HN  ))
  (( segid "BrD " and resid 21   and name HB  ))
     4.300      4.300      1.200 peak 10081 weight  0.10000E+01 volume  0.28058E+02 ppm1       8.666 ppm2       2.481
OR (10061)
  (( segid "BrD " and resid 24   and name HN  ))
  (( segid "BrD " and resid 26   and name HB1 ))
ASSI (10181)
  (( segid "BrD " and resid 16   and name HN  ))
  (( segid "BrD " and resid 14   and name HB2 ))
     4.100      4.100      1.400 peak 10181 weight  0.10000E+01 volume  0.40626E+02 ppm1       8.785 ppm2       2.129
OR (10181)
  (( segid "BrD " and resid 16   and name HN  ))
  (( segid "BrD " and resid 18   and name HB1 ))
ASSI (10201)
  (( segid "BrD " and resid 16   and name HN  ))
  (( segid "BrD " and resid 19   and name HB2 ))
     3.900      3.800      1.600 peak 10201 weight  0.10000E+01 volume  0.57921E+02 ppm1       8.791 ppm2       1.963
OR (10201)
  (( segid "BrD " and resid 16   and name HN  ))
  (( segid "BrD " and resid 113  and name HB% )
ASSI (10241)
  (( segid "BrD " and resid 75   and name HN  ))
  (( segid "BrD " and resid 78   and name HB1 ))
     3.900      3.800      1.600 peak 10241 weight  0.10000E+01 volume  0.50050E+02 ppm1       9.106 ppm2       1.347
OR (10241)
  (( segid "BrD " and resid 75   and name HN  ))
  (  segid "BrD " and resid 115  and name HD1%)
ASSI (10281)
  (( segid "BrD " and resid 98   and name HN  ))
  (( segid "BrD " and resid 97   and name HG1 ))
     4.000      4.000      1.500 peak 10281 weight  0.10000E+01 volume  0.43323E+02 ppm1       9.106 ppm2       2.456
OR (10281)
  (( segid "BrD " and resid 98   and name HN  ))
  (( segid "BrD " and resid 97   and name HD1 ))
OR (10281)
  (( segid "BrD " and resid 98   and name HN  ))
  (( segid "BrD " and resid 101  and name HG11))
ASSI (10331)
  (( segid "BrD " and resid 96   and name HN  ))
  (( segid "BrD " and resid 97   and name HG1 ))
     3.900      3.800      1.600 peak 10331 weight  0.10000E+01 volume  0.52265E+02 ppm1       7.977 ppm2       2.412
OR (10331)
  (( segid "BrD " and resid 77   and name HN  ))
  (( segid "BrD " and resid 73   and name HG  ))
OR (10331)
  (( segid "BrD " and resid 96   and name HN  ))
  (( segid "BrD " and resid 97   and name HD1 ))
OR (10331)
  (( segid "BrD " and resid 77   and name HN  ))
  (( segid "BrD " and resid 72   and name HB1 ))
ASSI (10381)
  (( segid "BrD " and resid 78   and name HN  ))
  (( segid "BrD " and resid 116  and name HG11))
     3.900      3.800      1.600 peak 10381 weight  0.10000E+01 volume  0.51654E+02 ppm1       7.996 ppm2       1.888
OR (10381)
  (( segid "BrD " and resid 77   and name HN  ))
  (( segid "BrD " and resid 116  and name HG11))
ASSI (10391)
  (( segid "BrD " and resid 78   and name HN  ))
  (  segid "BrD " and resid 22   and name HD2%)
     3.500      3.100      2.000 peak 10391 weight  0.10000E+01 volume  0.99200E+02 ppm1       7.996 ppm2       1.604
OR (10391)
  (( segid "BrD " and resid 55   and name HN  ))
  (  segid "BrD " and resid 22   and name HD2%)
OR (10391)
  (( segid "BrD " and resid 78   and name HN  ))
  (  segid "BrD " and resid 25   and name HG2%)
OR (10391)
  (( segid "BrD " and resid 77   and name HN  ))
  (  segid "BrD " and resid 22   and name HD2%)
OR (10391)
  (( segid "BrD " and resid 55   and name HN  ))
  (  segid "BrD " and resid 25   and name HG2%)
ASSI (10411)
  (( segid "BrD " and resid 77   and name HN  ))
  (( segid "BrD " and resid 80   and name HB2 ))
     2.800      2.000      2.000 peak 10411 weight  0.10000E+01 volume  0.43395E+03 ppm1       7.996 ppm2       2.456
OR (10411)
  (( segid "BrD " and resid 78   and name HN  ))
  (( segid "BrD " and resid 80   and name HB2 ))
ASSI (10431)
  (( segid "BrD " and resid 55   and name HN  ))
  (( segid "BrD " and resid 37   and name HG1 ))
     2.600      1.700      1.700 peak 10431 weight  0.10000E+01 volume  0.60264E+03 ppm1       7.996 ppm2       2.722
OR (10431)
  (( segid "BrD " and resid 78   and name HN  ))
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   (( segid "BrD " and resid 79   and name HB2 ))
ASSI (10471)
   (( segid "BrD " and resid 96   and name HN  ))
   (( segid "BrD " and resid 94   and name HA  ))
      3.900      3.800      1.600 peak 10471 weight  0.10000E+01 volume  0.52287E+02 ppm1       7.984 ppm2       4.814
OR (10471)
   (( segid "BrD " and resid 96   and name HN  ))
   (( segid "BrD " and resid 46   and name HA  ))
OR (10471)
   (( segid "BrD " and resid 96   and name HN  ))
   (( segid "BrD " and resid 92   and name HA  ))
ASSI (10501)
   (( segid "BrD " and resid 80   and name HN  ))
   (( segid "BrD " and resid 80   and name HA  ))
      2.800      2.000      2.000 peak 10501 weight  0.10000E+01 volume  0.42726E+03 ppm1       7.974 ppm2       4.691
OR (10501)
   (( segid "BrD " and resid 80   and name HN  ))
   (( segid "BrD " and resid 76   and name HA  ))
ASSI (10541)
   (( segid "BrD " and resid 55   and name HN  ))
   (  segid "BrD " and resid 58   and name HG2%)
      3.500      3.100      2.000 peak 10541 weight  0.10000E+01 volume  0.11084E+03 ppm1       7.974 ppm2       1.670
OR (10541)
   (( segid "BrD " and resid 78   and name HN  ))
   (  segid "BrD " and resid 22   and name HD1%)
OR (10541)
   (( segid "BrD " and resid 78   and name HN  ))
   (( segid "BrD " and resid 110  and name HG12))
OR (10541)
   (( segid "BrD " and resid 55   and name HN  ))
   (  segid "BrD " and resid 43   and name HB% )
OR (10541)
   (( segid "BrD " and resid 78   and name HN  ))
   (  segid "BrD " and resid 25   and name HG2%)
OR (10541)
   (( segid "BrD " and resid 55   and name HN  ))
   (  segid "BrD " and resid 25   and name HG2%)
OR (10541)
   (( segid "BrD " and resid 78   and name HN  ))
   (  segid "BrD " and resid 63   and name HD1%)
OR (10541)
   (( segid "BrD " and resid 55   and name HN  ))
   (  segid "BrD " and resid 22   and name HD1%)
ASSI (10551)
   (( segid "BrD " and resid 78   and name HN  ))
   (( segid "BrD " and resid 78   and name HB2 ))
      3.400      2.900      2.100 peak 10551 weight  0.10000E+01 volume  0.13253E+03 ppm1       7.975 ppm2       1.068
OR (10551)
   (( segid "BrD " and resid 80   and name HN  ))
   (  segid "BrD " and resid 81   and name HG1%)
OR (10551)
   (( segid "BrD " and resid 78   and name HN  ))
   (  segid "BrD " and resid 81   and name HG1%)
OR (10551)
   (( segid "BrD " and resid 55   and name HN  ))
   (  segid "BrD " and resid 81   and name HG1%)
ASSI (10611)
   (( segid "BrD " and resid 56   and name HN  ))
   (( segid "BrD " and resid 34   and name HB2 ))
      3.100      2.400      2.400 peak 10611 weight  0.10000E+01 volume  0.21458E+03 ppm1       9.680 ppm2       3.118
OR (10611)
   (( segid "BrD " and resid 56   and name HN  ))
   (( segid "BrD " and resid 59   and name HG2 ))
ASSI (10631)
   (( segid "BrD " and resid 82   and name HN  ))
   (  segid "BrD " and resid 83   and name HG2%)
      3.500      3.100      2.000 peak 10631 weight  0.10000E+01 volume  0.97408E+02 ppm1       6.981 ppm2       1.909
OR (10631)
   (( segid "BrD " and resid 82   and name HN  ))
   (( segid "BrD " and resid 103  and name HB2 ))
ASSI (10781)
   (( segid "BrD " and resid 80   and name HN  ))
   (  segid "BrD " and resid 83   and name HG2%)
      3.900      3.800      1.600 peak 10781 weight  0.10000E+01 volume  0.57791E+02 ppm1       8.006 ppm2       1.932
OR (10781)
   (( segid "BrD " and resid 80   and name HN  ))
   (( segid "BrD " and resid 116  and name HG11))
OR (10781)
   (( segid "BrD " and resid 80   and name HN  ))
   (( segid "BrD " and resid 54   and name HB2 ))
ASSI (10811)
   (( segid "BrD " and resid 80   and name HN  ))
   (  segid "BrD " and resid 81   and name HG1%)
      3.600      3.200      1.900 peak 10811 weight  0.10000E+01 volume  0.94805E+02 ppm1       8.005 ppm2       1.064
OR (10811)
   (( segid "BrD " and resid 80   and name HN  ))
   (( segid "BrD " and resid 78   and name HB2 ))
ASSI (10901)
   (( segid "BrD " and resid 85   and name HN  ))
   (( segid "BrD " and resid 86   and name HG1 ))
      3.800      3.600      1.700 peak 10901 weight  0.10000E+01 volume  0.64876E+02 ppm1       7.516 ppm2       1.905
OR (10901)
   (( segid "BrD " and resid 85   and name HN  ))
   (  segid "BrD " and resid 83   and name HG2%)
ASSI (10981)
   (( segid "BrD " and resid 87   and name HN  ))
   (( segid "BrD " and resid 85   and name HA  ))
      3.900      3.800      1.600 peak 10981 weight  0.10000E+01 volume  0.57856E+02 ppm1       8.572 ppm2       5.005
OR (10981)
   (( segid "BrD " and resid 87   and name HN  ))
   (( segid "BrD " and resid 88   and name HA  ))
ASSI (10991)
   (( segid "BrD " and resid 87   and name HN  ))
   (( segid "BrD " and resid 85   and name HB2 ))
      3.200      2.600      2.300 peak 10991 weight  0.10000E+01 volume  0.17351E+03 ppm1       8.571 ppm2       3.639
OR (10991)
   (( segid "BrD " and resid 87   and name HN  ))
   (( segid "BrD " and resid 95   and name HB1 ))
ASSI (11181)
   (( segid "BrD " and resid 93   and name HN  ))
   (( segid "BrD " and resid 91   and name HB1 ))
      3.000      2.200      2.200 peak 11181 weight  0.10000E+01 volume  0.28245E+03 ppm1       8.714 ppm2       3.075
OR (11181)
   (( segid "BrD " and resid 93   and name HN  ))
   (( segid "BrD " and resid 96   and name HB2 ))
ASSI (11231)
   (( segid "BrD " and resid 31   and name HN  ))
   (( segid "BrD " and resid 98   and name HB1 ))
      3.900      3.800      1.600 peak 11231 weight  0.10000E+01 volume  0.56370E+02 ppm1       8.481 ppm2       3.992
OR (11231)
   (( segid "BrD " and resid 31   and name HN  ))
   (( segid "BrD " and resid 32   and name HB2 ))
ASSI (11271)
   (( segid "BrD " and resid 31   and name HN  ))
   (( segid "BrD " and resid 33   and name HD1 ))
      4.100      4.100      1.400 peak 11271 weight  0.10000E+01 volume  0.42900E+02 ppm1       8.480 ppm2       2.781
OR (11271)
   (( segid "BrD " and resid 59   and name HN  ))
   (( segid "BrD " and resid 61   and name HG2 ))
ASSI (11301)
   (( segid "BrD " and resid 31   and name HN  ))
   (  segid "BrD " and resid 101  and name HD1%)
      3.800      3.600      1.700 peak 11301 weight  0.10000E+01 volume  0.60718E+02 ppm1       8.479 ppm2       1.542
OR (11301)
   (( segid "BrD " and resid 31   and name HN  ))
   (  segid "BrD " and resid 56   and name HD1%)
ASSI (11321)
   (( segid "BrD " and resid 59   and name HN  ))
   (  segid "BrD " and resid 81   and name HG1%)
      4.200      4.200      1.300 peak 11321 weight  0.10000E+01 volume  0.33324E+02 ppm1       8.480 ppm2       1.110
OR (11321)
   (( segid "BrD " and resid 31   and name HN  ))
   (( segid "BrD " and resid 33   and name HB1 ))
ASSI (11531)
   (( segid "BrD " and resid 104  and name HN  ))
   (  segid "BrD " and resid 102  and name HD2%)
      4.700      4.700      0.800 peak 11531 weight  0.10000E+01 volume  0.16001E+02 ppm1       7.735 ppm2       1.282
OR (11531)
   (( segid "BrD " and resid 35   and name HN  ))
   (  segid "BrD " and resid 102  and name HD1%)
OR (11531)
   (( segid "BrD " and resid 104  and name HN  ))
   (  segid "BrD " and resid 102  and name HD1%)
ASSI (11541)
   (( segid "BrD " and resid 35   and name HN  ))
   (( segid "BrD " and resid 32   and name HB2 ))
      3.400      2.900      2.100 peak 11541 weight  0.10000E+01 volume  0.13237E+03 ppm1       7.734 ppm2       3.923
OR (11541)
   (( segid "BrD " and resid 104  and name HN  ))
   (( segid "BrD " and resid 106  and name HB1 ))
ASSI (11591)
   (( segid "BrD " and resid 66   and name HN  ))
   (( segid "BrD " and resid 69   and name HB  ))
      3.600      3.200      1.900 peak 11591 weight  0.10000E+01 volume  0.90637E+02 ppm1       8.764 ppm2       2.935
OR (11591)
   (( segid "BrD " and resid 66   and name HN  ))
   (( segid "BrD " and resid 63   and name HB1 ))
ASSI (11631)
   (( segid "BrD " and resid 67   and name HN  ))
   (  segid "BrD " and resid 63   and name HD1%)
      3.500      3.100      2.000 peak 11631 weight  0.10000E+01 volume  0.95713E+02 ppm1       8.832 ppm2       1.678
OR (11631)
   (( segid "BrD " and resid 67   and name HN  ))
   (( segid "BrD " and resid 62   and name HB2 ))
ASSI (11671)
   (( segid "BrD " and resid 68   and name HN  ))
   (  segid "BrD " and resid 63   and name HD1%)
      3.600      3.200      1.900 peak 11671 weight  0.10000E+01 volume  0.92729E+02 ppm1       8.626 ppm2       1.684
OR (11671)
   (( segid "BrD " and resid 68   and name HN  ))
   (( segid "BrD " and resid 62   and name HB2 ))
ASSI (11701)
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   (( segid "BrD " and resid 69   and name HN  ))
   (( segid "BrD " and resid 63   and name HG  ))
      3.400      2.900      2.100 peak 11701 weight  0.10000E+01 volume  0.12326E+03 ppm1      8.306 ppm2      2.476
OR (11701)
   (( segid "BrD " and resid 69   and name HN  ))
   (( segid "BrD " and resid 73   and name HB2 ))
ASSI (11711)
   (( segid "BrD " and resid 69   and name HN  ))
   (( segid "BrD " and resid 66   and name HB2 ))
      3.800      3.600      1.700 peak 11711 weight  0.10000E+01 volume  0.68030E+02 ppm1      8.306 ppm2      2.614
OR (11711)
   (( segid "BrD " and resid 69   and name HN  ))
   (( segid "BrD " and resid 11   and name HB2 ))
OR (11711)
   (( segid "BrD " and resid 69   and name HN  ))
   (( segid "BrD " and resid 73   and name HB1 ))
ASSI (11751)
   (( segid "BrD " and resid 70   and name HN  ))
   (( segid "BrD " and resid 73   and name HG  ))
      4.200      4.200      1.300 peak 11751 weight  0.10000E+01 volume  0.36902E+02 ppm1      8.039 ppm2      2.374
OR (11751)
   (( segid "BrD " and resid 70   and name HN  ))
   (( segid "BrD " and resid 9    and name HB2 ))
ASSI (11761)
   (( segid "BrD " and resid 70   and name HN  ))
   (( segid "BrD " and resid 73   and name HB1 ))
      3.500      3.100      2.000 peak 11761 weight  0.10000E+01 volume  0.95470E+02 ppm1      8.040 ppm2      2.594
OR (11761)
   (( segid "BrD " and resid 70   and name HN  ))
   (( segid "BrD " and resid 11   and name HB2 ))
ASSI (11851)
   (( segid "BrD " and resid 73   and name HN  ))
   (( segid "BrD " and resid 74   and name HB1 ))
      3.600      3.200      1.900 peak 11851 weight  0.10000E+01 volume  0.82682E+02 ppm1      8.045 ppm2      3.572
OR (11851)
   (( segid "BrD " and resid 73   and name HN  ))
   (( segid "BrD " and resid 75   and name HG1 ))
ASSI (11931)
   (( segid "BrD " and resid 23   and name HN  ))
   (( segid "BrD " and resid 22   and name HA  ))
      3.800      3.600      1.700 peak 11931 weight  0.10000E+01 volume  0.64947E+02 ppm1      9.125 ppm2      4.688
OR (11931)
   (( segid "BrD " and resid 75   and name HN  ))
   (( segid "BrD " and resid 72   and name HA  ))
ASSI (11941)
   (( segid "BrD " and resid 98   and name HN  ))
   (( segid "BrD " and resid 100  and name HB2 ))
      4.000      4.000      1.500 peak 11941 weight  0.10000E+01 volume  0.47235E+02 ppm1      9.125 ppm2      3.411
OR (11941)
   (( segid "BrD " and resid 23   and name HN  ))
   (( segid "BrD " and resid 24   and name HG1 ))
ASSI (12011)
   (( segid "BrD " and resid 23   and name HN  ))
   (  segid "BrD " and resid 22   and name HD2#)
      3.800      3.600      1.700 peak 12011 weight  0.10000E+01 volume  0.60527E+02 ppm1      9.125 ppm2      1.594
OR (12011)
   (( segid "BrD " and resid 23   and name HN  ))
   (  segid "BrD " and resid 21   and name HG2#)
ASSI (12021)
   (( segid "BrD " and resid 98   and name HN  ))
   (( segid "BrD " and resid 30   and name HB1 ))
      4.000      4.000      1.500 peak 12021 weight  0.10000E+01 volume  0.46966E+02 ppm1      9.124 ppm2      4.936
OR (12021)
   (( segid "BrD " and resid 23   and name HN  ))
   (( segid "BrD " and resid 60   and name HB1 ))
OR (12021)
   (( segid "BrD " and resid 98   and name HN  ))
   (( segid "BrD " and resid 100  and name HA  ))
OR (12021)
   (( segid "BrD " and resid 23   and name HN  ))
   (( segid "BrD " and resid 64   and name HA  ))
ASSI (12071)
   (( segid "BrD " and resid 100  and name HN  ))
   (( segid "BrD " and resid 98   and name HB2 ))
      4.100      4.100      1.400 peak 12071 weight  0.10000E+01 volume  0.37827E+02 ppm1      8.669 ppm2      3.641
OR (12071)
   (( segid "BrD " and resid 100  and name HN  ))
   (( segid "BrD " and resid 65   and name HB2 ))
ASSI (12101)
   (( segid "BrD " and resid 100  and name HN  ))
   (( segid "BrD " and resid 103  and name HB1 ))
      2.000      2.000      2.500 peak 12101 weight  0.10000E+01 volume  0.26537E+04 ppm1      8.669 ppm2      2.323
OR (12101)
   (( segid "BrD " and resid 100  and name HN  ))
   (( segid "BrD " and resid 104  and name HD1 ))
ASSI (12111)
   (( segid "BrD " and resid 100  and name HN  ))
   (( segid "BrD " and resid 103  and name HB2 ))
      4.100      4.100      1.400 peak 12111 weight  0.10000E+01 volume  0.37921E+02 ppm1      8.669 ppm2      1.892
OR (12111)
   (( segid "BrD " and resid 100  and name HN  ))
   (( segid "BrD " and resid 86   and name HG1 ))
ASSI (12141)
   (( segid "BrD " and resid 100  and name HN  ))
   (  segid "BrD " and resid 96   and name HD% )
      4.300      4.300      1.200 peak 12141 weight  0.10000E+01 volume  0.30609E+02 ppm1      8.669 ppm2      7.737
OR (12141)
   (( segid "BrD " and resid 100  and name HN  ))
   (( segid "BrD " and resid 104  and name HN  ))
ASSI (12251)
   (( segid "BrD " and resid 107  and name HN  ))
   (( segid "BrD " and resid 110  and name HB  ))
      3.700      3.400      1.800 peak 12251 weight  0.10000E+01 volume  0.79191E+02 ppm1      8.980 ppm2      2.348
OR (12251)
   (( segid "BrD " and resid 107  and name HN  ))
   (( segid "BrD " and resid 103  and name HB1 ))
OR (12251)
   (( segid "BrD " and resid 107  and name HN  ))
   (( segid "BrD " and resid 109  and name HB1 ))
ASSI (12261)
   (( segid "BrD " and resid 107  and name HN  ))
   (( segid "BrD " and resid 102  and name HB2 ))
      5.500      5.500      0.000 peak 12261 weight  0.10000E+01 volume  0.35919E+00 ppm1      8.980 ppm2      1.797
OR (12261)
   (( segid "BrD " and resid 107  and name HN  ))
   (  segid "BrD " and resid 25   and name HG1#)
ASSI (12281)
   (( segid "BrD " and resid 108  and name HN  ))
   (( segid "BrD " and resid 102  and name HG2 ))
      4.100      4.100      1.400 peak 12281 weight  0.10000E+01 volume  0.42059E+02 ppm1      8.522 ppm2      2.529
OR (12281)
   (( segid "BrD " and resid 108  and name HN  ))
   (( segid "BrD " and resid 104  and name HB1 ))
ASSI (12301)
   (( segid "BrD " and resid 108  and name HN  ))
   (  segid "BrD " and resid 116  and name HD1#)
      3.900      3.800      1.600 peak 12301 weight  0.10000E+01 volume  0.52230E+02 ppm1      8.521 ppm2      1.422
OR (12301)
   (( segid "BrD " and resid 108  and name HN  ))
   (( segid "BrD " and resid 109  and name HG1 ))
ASSI (12311)
   (( segid "BrD " and resid 108  and name HN  ))
   (( segid "BrD " and resid 110  and name HB  ))
      4.100      4.100      1.400 peak 12311 weight  0.10000E+01 volume  0.41867E+02 ppm1      8.522 ppm2      2.331
OR (12311)
   (( segid "BrD " and resid 108  and name HN  ))
   (( segid "BrD " and resid 109  and name HB1 ))
ASSI (12401)
   (( segid "BrD " and resid 113  and name HN  ))
   (( segid "BrD " and resid 115  and name HG  ))
      3.300      2.700      2.200 peak 12401 weight  0.10000E+01 volume  0.16014E+03 ppm1      8.218 ppm2      2.152
OR (12401)
   (( segid "BrD " and resid 113  and name HN  ))
   (( segid "BrD " and resid 115  and name HB1 ))
OR (12401)
   (( segid "BrD " and resid 113  and name HN  ))
   (( segid "BrD " and resid 109  and name HB2 ))
ASSI (12501)
   (( segid "BrD " and resid 116  and name HN  ))
   (( segid "BrD " and resid 71   and name HA  ))
      4.300      4.300      1.200 peak 12501 weight  0.10000E+01 volume  0.28782E+02 ppm1      8.087 ppm2      4.664
OR (12501)
   (( segid "BrD " and resid 116  and name HN  ))
   (( segid "BrD " and resid 72   and name HA  ))
OR (12501)
   (( segid "BrD " and resid 116  and name HN  ))
   (( segid "BrD " and resid 114  and name HA1 ))
OR (12501)
   (( segid "BrD " and resid 116  and name HN  ))
   (( segid "BrD " and resid 76   and name HA  ))
ASSI (12511)
   (( segid "BrD " and resid 116  and name HN  ))
   (( segid "BrD " and resid 75   and name HA  ))
      3.600      3.200      1.900 peak 12511 weight  0.10000E+01 volume  0.81005E+02 ppm1      8.087 ppm2      4.526
OR (12511)
   (( segid "BrD " and resid 116  and name HN  ))
   (( segid "BrD " and resid 114  and name HA2 ))
ASSI (12601)
   (( segid "BrD " and resid 92   and name HN  ))
   (( segid "BrD " and resid 92   and name HB1 ))
      4.100      4.100      1.400 peak 12601 weight  0.10000E+01 volume  0.37922E+02 ppm1      8.831 ppm2      2.695
OR (12601)
   (( segid "BrD " and resid 92   and name HN  ))
   (( segid "BrD " and resid 91   and name HB2 ))
ASSI (12841)
   (( segid "BrD " and resid 19   and name HN  ))
   (( segid "BrD " and resid 17   and name HB  ))
      3.800      3.600      1.700 peak 12841 weight  0.10000E+01 volume  0.59211E+02 ppm1      9.187 ppm2      4.880
OR (12841)
   (( segid "BrD " and resid 19   and name HN  ))
   (( segid "BrD " and resid 20   and name HA  ))
ASSI (12861)
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   (( segid "BrD " and resid 20   and name HN  ))
   (( segid "BrD " and resid 63   and name HG  ))
     4.000      4.000      1.500 peak 12861 weight  0.10000E+01 volume  0.43415E+02 ppm1       8.147 ppm2       2.471
OR (12861)
   (( segid "BrD " and resid 20   and name HN  ))
   (( segid "BrD " and resid 21   and name HB  ))
ASSI (12951)
   (( segid "BrD " and resid 23   and name HN  ))
   (  segid "BrD " and resid 25   and name HG1%)
     3.800      3.600      1.700 peak 12951 weight  0.10000E+01 volume  0.65898E+02 ppm1       9.119 ppm2       1.823
OR (12951)
   (( segid "BrD " and resid 98   and name HN  ))
   (( segid "BrD " and resid 101  and name HG12))
ASSI (12961)
   (( segid "BrD " and resid 23   and name HN  ))
   (  segid "BrD " and resid 22   and name HD1%)
     3.100      2.400      2.400 peak 12961 weight  0.10000E+01 volume  0.23452E+03 ppm1       9.120 ppm2       1.646
OR (12961)
   (( segid "BrD " and resid 23   and name HN  ))
   (( segid "BrD " and resid 21   and name HG12))
OR (12961)
   (( segid "BrD " and resid 23   and name HN  ))
   (  segid "BrD " and resid 21   and name HG2%)
OR (12961)
   (( segid "BrD " and resid 23   and name HN  ))
   (  segid "BrD " and resid 25   and name HG2%)
ASSI (12971)
   (( segid "BrD " and resid 98   and name HN  ))
   (  segid "BrD " and resid 101  and name HD1%)
     3.900      3.800      1.600 peak 12971 weight  0.10000E+01 volume  0.50522E+02 ppm1       9.119 ppm2       1.514
OR (12971)
   (( segid "BrD " and resid 23   and name HN  ))
   (  segid "BrD " and resid 63   and name HD2%)
ASSI (12981)
   (( segid "BrD " and resid 98   and name HN  ))
   (( segid "BrD " and resid 100  and name HB2 ))
     3.400      2.900      2.100 peak 12981 weight  0.10000E+01 volume  0.12055E+03 ppm1       9.119 ppm2       3.467
OR (12981)
   (( segid "BrD " and resid 23   and name HN  ))
   (( segid "BrD " and resid 24   and name HG1 ))
OR (12981)
   (( segid "BrD " and resid 98   and name HN  ))
   (( segid "BrD " and resid 100  and name HB1 ))
ASSI (13001)
   (( segid "BrD " and resid 98   and name HN  ))
   (  segid "BrD " and resid 95   and name HD% )
     3.900      3.800      1.600 peak 13001 weight  0.10000E+01 volume  0.54095E+02 ppm1       9.119 ppm2       7.520
OR (13001)
   (( segid "BrD " and resid 23   and name HN  ))
   (( segid "BrD " and resid 24   and name HE22))
OR (13001)
   (( segid "BrD " and resid 23   and name HN  ))
   (  segid "BrD " and resid 74   and name HE% )
ASSI (13011)
   (( segid "BrD " and resid 26   and name HN  ))
   (  segid "BrD " and resid 31   and name HB% )
     3.500      3.100      2.000 peak 13011 weight  0.10000E+01 volume  0.10060E+03 ppm1       9.196 ppm2       2.308
OR (13011)
   (( segid "BrD " and resid 26   and name HN  ))
   (( segid "BrD " and resid 22   and name HB2 ))
ASSI (13121)
   (( segid "BrD " and resid 59   and name HN  ))
   (( segid "BrD " and resid 56   and name HB2 ))
     3.800      3.600      1.700 peak 13121 weight  0.10000E+01 volume  0.59266E+02 ppm1       8.496 ppm2       2.008
OR (13121)
   (( segid "BrD " and resid 59   and name HN  ))
   (( segid "BrD " and resid 57   and name HG2 ))
OR (13121)
   (( segid "BrD " and resid 31   and name HN  ))
   (( segid "BrD " and resid 102  and name HB1 ))
ASSI (13171)
   (( segid "BrD " and resid 60   and name HN  ))
   (( segid "BrD " and resid 57   and name HB2 ))
     3.500      3.100      2.000 peak 13171 weight  0.10000E+01 volume  0.10295E+03 ppm1       8.564 ppm2       2.858
OR (13171)
   (( segid "BrD " and resid 60   and name HN  ))
   (( segid "BrD " and resid 61   and name HB1 ))
OR (13171)
   (( segid "BrD " and resid 65   and name HN  ))
   (( segid "BrD " and resid 61   and name HB1 ))
ASSI (13181)
   (( segid "BrD " and resid 60   and name HN  ))
   (( segid "BrD " and resid 22   and name HG  ))
     3.800      3.600      1.700 peak 13181 weight  0.10000E+01 volume  0.61364E+02 ppm1       8.565 ppm2       2.336
OR (13181)
   (( segid "BrD " and resid 65   and name HN  ))
   (( segid "BrD " and resid 62   and name HG1 ))
OR (13181)
   (( segid "BrD " and resid 60   and name HN  ))
   (( segid "BrD " and resid 56   and name HG  ))
OR (13181)
   (( segid "BrD " and resid 60   and name HN  ))
   (( segid "BrD " and resid 22   and name HB2 ))
OR (13181)
   (( segid "BrD " and resid 60   and name HN  ))
   (( segid "BrD " and resid 57   and name HD2 ))
ASSI (13191)
   (( segid "BrD " and resid 60   and name HN  ))
   (  segid "BrD " and resid 22   and name HD1%)
     3.200      2.600      2.300 peak 13191 weight  0.10000E+01 volume  0.17809E+03 ppm1       8.568 ppm2       1.666
OR (13191)
   (( segid "BrD " and resid 65   and name HN  ))
   (  segid "BrD " and resid 63   and name HD1%)
OR (13191)
   (( segid "BrD " and resid 60   and name HN  ))
   (  segid "BrD " and resid 58   and name HG2%)
ASSI (13201)
   (( segid "BrD " and resid 65   and name HN  ))
   (  segid "BrD " and resid 63   and name HD2%)
     3.600      3.200      1.900 peak 13201 weight  0.10000E+01 volume  0.81304E+02 ppm1       8.565 ppm2       1.497
OR (13201)
   (( segid "BrD " and resid 65   and name HN  ))
   (( segid "BrD " and resid 62   and name HG2 ))
OR (13201)
   (( segid "BrD " and resid 60   and name HN  ))
   (  segid "BrD " and resid 63   and name HD2%)
ASSI (13631)
   (( segid "BrD " and resid 84   and name HN  ))
   (( segid "BrD " and resid 82   and name HN  ))
     4.000      4.000      1.500 peak 13631 weight  0.10000E+01 volume  0.44090E+02 ppm1       9.463 ppm2       6.981
OR (13631)
   (( segid "BrD " and resid 63   and name HN  ))
   (  segid "BrD " and resid 74   and name HD% )
ASSI (13691)
   (( segid "BrD " and resid 22   and name HN  ))
   (( segid "BrD " and resid 22   and name HB2 ))
     3.700      3.400      1.800 peak 13691 weight  0.10000E+01 volume  0.68908E+02 ppm1       9.473 ppm2       2.333
OR (13691)
   (( segid "BrD " and resid 22   and name HN  ))
   (( segid "BrD " and resid 21   and name HG11))
OR (13691)
   (( segid "BrD " and resid 22   and name HN  ))
   (( segid "BrD " and resid 22   and name HG  ))
ASSI (13971)
   (( segid "BrD " and resid 114  and name HN  ))
   (( segid "BrD " and resid 112  and name HG2 ))
     4.900      4.900      0.600 peak 13971 weight  0.10000E+01 volume  0.14459E+02 ppm1       8.377 ppm2       2.786
OR (13971)
   (( segid "BrD " and resid 114  and name HN  ))
   (( segid "BrD " and resid 13   and name HB1 ))
ASSI (14061)
   (( segid "BrD " and resid 107  and name HN  ))
   (  segid "BrD " and resid 110  and name HG2%)
     4.800      4.800      0.700 peak 14061 weight  0.10000E+01 volume  0.15271E+02 ppm1       8.980 ppm2       1.260
OR (14061)
   (( segid "BrD " and resid 107  and name HN  ))
   (  segid "BrD " and resid 21   and name HD1%)
ASSI (14071)
   (( segid "BrD " and resid 106  and name HN  ))
   (( segid "BrD " and resid 107  and name HA  ))
     4.600      4.600      0.900 peak 14071 weight  0.10000E+01 volume  0.20679E+02 ppm1       9.742 ppm2       4.447
OR (14071)
   (( segid "BrD " and resid 106  and name HN  ))
   (( segid "BrD " and resid 99   and name HA  ))
ASSI (14131)
   (( segid "BrD " and resid 104  and name HN  ))
   (( segid "BrD " and resid 102  and name HB2 ))
     3.700      3.400      1.800 peak 14131 weight  0.10000E+01 volume  0.79648E+02 ppm1       7.763 ppm2       1.816
OR (14131)
   (( segid "BrD " and resid 104  and name HN  ))
   (( segid "BrD " and resid 101  and name HG12))
ASSI (14161)
   (( segid "BrD " and resid 103  and name HN  ))
   (( segid "BrD " and resid 106  and name HB1 ))
     3.600      3.200      1.900 peak 14141 weight  0.10000E+01 volume  0.92105E+02 ppm1       8.695 ppm2       3.908
OR (14161)
   (( segid "BrD " and resid 17   and name HN  ))
   (( segid "BrD " and resid 18   and name HA  ))
ASSI (14151)
   (( segid "BrD " and resid 102  and name HN  ))
   (( segid "BrD " and resid 105  and name HB2 ))
     4.000      4.000      1.500 peak 14151 weight  0.10000E+01 volume  0.49406E+02 ppm1       9.156 ppm2       3.635
OR (14151)
   (( segid "BrD " and resid 102  and name HN  ))
   (( segid "BrD " and resid 98   and name HB2 ))
OR (14151)
   (( segid "BrD " and resid 102  and name HN  ))
   (( segid "BrD " and resid 106  and name HB2 ))
ASSI (14161)
   (( segid "BrD " and resid 102  and name HN  ))
   (( segid "BrD " and resid 103  and name HA  ))
     5.000      5.000      0.500 peak 14161 weight  0.10000E+01 volume  0.12711E+02 ppm1       9.156 ppm2       3.783
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OR (14161)
  (( segid "BrD " and resid 102  and name HN  ))
  (( segid "BrD " and resid 105  and name HB1 ))
ASSI (14171)
  (( segid "BrD " and resid 101  and name HN  ))
  (( segid "BrD " and resid 104  and name HN  ))
     4.300      4.100      1.200 peak 14171 weight  0.10000E+01 volume  0.29353E+02 ppm1      8.513 ppm2      7.761
OR (14171)
  (( segid "BrD " and resid 101  and name HN  ))
  (  segid "BrD " and resid 34   and name HE% )
ASSI (14201)
  (( segid "BrD " and resid 100  and name HN  ))
  (( segid "BrD " and resid 86   and name HE1 ))
     4.100      4.100      1.400 peak 14201 weight  0.10000E+01 volume  0.38990E+02 ppm1      8.667 ppm2      3.092
OR (14201)
  (( segid "BrD " and resid 100  and name HN  ))
  (( segid "BrD " and resid 96   and name HB2 ))
ASSI (14221)
  (( segid "BrD " and resid 100  and name HN  ))
  (( segid "BrD " and resid 101  and name HG12))
     4.800      4.800      0.700 peak 14221 weight  0.10000E+01 volume  0.14931E+02 ppm1      8.669 ppm2      1.806
OR (14221)
  (( segid "BrD " and resid 100  and name HN  ))
  (( segid "BrD " and resid 102  and name HB2 ))
ASSI (14241)
  (( segid "BrD " and resid 99   and name HN  ))
  (( segid "BrD " and resid 96   and name HB2 ))
     4.900      4.900      0.600 peak 14241 weight  0.10000E+01 volume  0.14325E+02 ppm1      8.940 ppm2      3.103
OR (14241)
  (( segid "BrD " and resid 99   and name HN  ))
  (( segid "BrD " and resid 94   and name HG1 ))
OR (14241)
  (( segid "BrD " and resid 99   and name HN  ))
  (( segid "BrD " and resid 86   and name HE1 ))
ASSI (14251)
  (( segid "BrD " and resid 99   and name HN  ))
  (  segid "BrD " and resid 81   and name HG2% )
     5.500      5.500      0.000 peak 14251 weight  0.10000E+01 volume  0.30696E+01 ppm1      8.934 ppm2      0.748
OR (14251)
  (( segid "BrD " and resid 99   and name HN  ))
  (( segid "BrD " and resid 86   and name HG2 ))
ASSI (14281)
  (( segid "BrD " and resid 98   and name HN  ))
  (( segid "BrD " and resid 32   and name HN2 ))
     3.800      3.600      1.700 peak 14281 weight  0.10000E+01 volume  0.66237E+02 ppm1      9.125 ppm2      7.750
OR (14281)
  (( segid "BrD " and resid 98   and name HN  ))
  (  segid "BrD " and resid 34   and name HE% )
OR (14281)
  (( segid "BrD " and resid 75   and name HN  ))
  (  segid "BrD " and resid 68   and name HD% )
ASSI (14301)
  (( segid "BrD " and resid 96   and name HN  ))
  (  segid "BrD " and resid 99   and name HB% )
     3.600      3.200      1.900 peak 14301 weight  0.10000E+01 volume  0.84940E+02 ppm1      7.977 ppm2      2.199
OR (14301)
  (( segid "BrD " and resid 96   and name HN  ))
  (( segid "BrD " and resid 97   and name HG2 ))
ASSI (14311)
  (( segid "BrD " and resid 77   and name HN  ))
  (  segid "BrD " and resid 73   and name HD1% )
     4.900      4.900      0.600 peak 14311 weight  0.10000E+01 volume  0.13346E+02 ppm1      7.981 ppm2      1.543
OR (14311)
  (( segid "BrD " and resid 78   and name HN  ))
  (( segid "BrD " and resid 116  and name HG12))
OR (14311)
  (( segid "BrD " and resid 78   and name HN  ))
  (  segid "BrD " and resid 56   and name HD1% )
OR (14311)
  (( segid "BrD " and resid 77   and name HN  ))
  (( segid "BrD " and resid 116  and name HG12))
OR (14311)
  (( segid "BrD " and resid 96   and name HN  ))
  (  segid "BrD " and resid 101  and name HD1% )
ASSI (14441)
  (( segid "BrD " and resid 83   and name HN  ))
  (( segid "BrD " and resid 79   and name HG1 ))
     4.600      4.600      0.900 peak 14441 weight  0.10000E+01 volume  0.19968E+02 ppm1      9.658 ppm2      3.046
OR (14441)
  (( segid "BrD " and resid 83   and name HN  ))
  (( segid "BrD " and resid 87   and name HG1 ))
ASSI (14451)
  (( segid "BrD " and resid 83   and name HN  ))
  (( segid "BrD " and resid 80   and name HG1 ))
     5.500      5.500      0.000 peak 14451 weight  0.10000E+01 volume  0.45437E+00 ppm1      9.658 ppm2      2.374
OR (14451)
  (( segid "BrD " and resid 83   and name HN  ))
  (( segid "BrD " and resid 86   and name HB1 ))
ASSI (14461)
  (( segid "BrD " and resid 83   and name HN  ))
  (( segid "BrD " and resid 86   and name HG2 ))
     5.000      5.000      0.500 peak 14461 weight  0.10000E+01 volume  0.12633E+02 ppm1      9.657 ppm2      0.743
OR (14461)
  (( segid "BrD " and resid 83   and name HN  ))
  (  segid "BrD " and resid 81   and name HG2% )
ASSI (14511)
  (( segid "BrD " and resid 79   and name HN  ))
  (  segid "BrD " and resid 106  and name HE% )
     3.600      3.200      1.900 peak 14511 weight  0.10000E+01 volume  0.86513E+02 ppm1      8.680 ppm2      7.621
OR (14511)
  (( segid "BrD " and resid 79   and name HN  ))
  (( segid "BrD " and resid 81   and name HN  ))
ASSI (14591)
  (( segid "BrD " and resid 72   and name HN  ))
  (( segid "BrD " and resid 73   and name HA  ))
     4.100      4.100      1.400 peak 14591 weight  0.10000E+01 volume  0.40514E+02 ppm1      8.858 ppm2      4.801
OR (14591)
  (( segid "BrD " and resid 72   and name HN  ))
  (( segid "BrD " and resid 70   and name HB1 ))
OR (14591)
  (( segid "BrD " and resid 72   and name HN  ))
  (( segid "BrD " and resid 115  and name HA  ))
ASSI (14631)
  (( segid "BrD " and resid 66   and name HN  ))
  (( segid "BrD " and resid 67   and name HA  ))
     4.400      4.400      1.100 peak 14631 weight  0.10000E+01 volume  0.25627E+02 ppm1      8.762 ppm2      4.678
OR (14631)
  (( segid "BrD " and resid 66   and name HN  ))
  (( segid "BrD " and resid 69   and name HA  ))
OR (14631)
  (( segid "BrD " and resid 66   and name HN  ))
  (( segid "BrD " and resid 61   and name HA  ))
ASSI (14641)
  (( segid "BrD " and resid 60   and name HN  ))
  (( segid "BrD " and resid 62   and name HN  ))
     4.200      4.200      1.300 peak 14641 weight  0.10000E+01 volume  0.32935E+02 ppm1      8.568 ppm2      8.968
OR (14641)
  (( segid "BrD " and resid 65   and name HN  ))
  (( segid "BrD " and resid 62   and name HN  ))
ASSI (14651)
  (( segid "BrD " and resid 65   and name HN  ))
  (( segid "BrD " and resid 65   and name HD22))
     4.200      4.200      1.300 peak 14651 weight  0.10000E+01 volume  0.33097E+02 ppm1      8.566 ppm2      7.569
OR (14651)
  (( segid "BrD " and resid 60   and name HN  ))
  (  segid "BrD " and resid 74   and name HE% )
ASSI (14751)
  (( segid "BrD " and resid 62   and name HN  ))
  (( segid "BrD " and resid 64   and name HN  ))
     2.800      2.000      2.000 peak 14751 weight  0.10000E+01 volume  0.39545E+03 ppm1      8.998 ppm2      8.576
OR (14751)
  (( segid "BrD " and resid 62   and name HN  ))
  (( segid "BrD " and resid 60   and name HN  ))
ASSI (14791)
  (( segid "BrD " and resid 38   and name HN  ))
  (( segid "BrD " and resid 37   and name HG2 ))
     3.900      3.800      1.600 peak 14791 weight  0.10000E+01 volume  0.52365E+02 ppm1      8.742 ppm2      2.547
OR (14791)
  (( segid "BrD " and resid 61   and name HN  ))
  (  segid "BrD " and resid 54   and name HE% )
OR (14791)
  (( segid "BrD " and resid 61   and name HN  ))
  (( segid "BrD " and resid 59   and name HB2 ))
OR (14791)
  (( segid "BrD " and resid 61   and name HN  ))
  (( segid "BrD " and resid 63   and name HB2 ))
ASSI (14801)
  (( segid "BrD " and resid 65   and name HN  ))
  (( segid "BrD " and resid 63   and name HN  ))
     4.400      4.400      1.100 peak 14801 weight  0.10000E+01 volume  0.24650E+02 ppm1      8.570 ppm2      9.470
OR (14801)
  (( segid "BrD " and resid 60   and name HN  ))
  (( segid "BrD " and resid 63   and name HN  ))
ASSI (14821)
  (( segid "BrD " and resid 59   and name HN  ))
  (( segid "BrD " and resid 55   and name HN  ))
     3.600      3.200      1.900 peak 14821 weight  0.10000E+01 volume  0.84273E+02 ppm1      8.498 ppm2      7.974
OR (14821)
  (( segid "BrD " and resid 31   and name HN  ))
  (( segid "BrD " and resid 32   and name HE2 ))
ASSI (14901)
  (( segid "BrD " and resid 54   and name HN  ))
  (( segid "BrD " and resid 55   and name HB1 ))
     4.400      4.400      1.100 peak 14901 weight  0.10000E+01 volume  0.25948E+02 ppm1      9.035 ppm2      2.965
OR (14901)
  (( segid "BrD " and resid 54   and name HN  ))
  (( segid "BrD " and resid 37   and name HB1 ))
ASSI (14921)
  (( segid "BrD " and resid 54   and name HN  ))
  (  segid "BrD " and resid 81   and name HG1% )
     4.000      4.000      1.500 peak 14921 weight  0.10000E+01 volume  0.46525E+02 ppm1      9.037 ppm2      1.081
OR (14921)
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  (( segid "BrD " and resid 54   and name HN  ))
  (  segid "BrD " and resid 38   and name HG1%)
ASSI (14931)
  (( segid "BrD " and resid 52   and name HN  ))
  (  segid "BrD " and resid 50   and name HD1%)
    5.500      5.500      0.000 peak 14931 weight  0.10000E+01 volume  0.20319E+01 ppm1      9.004 ppm2      1.110
OR (14931)
  (( segid "BrD " and resid 52   and name HN  ))
  (  segid "BrD " and resid 81   and name HG1%)
ASSI (15021)
  (( segid "BrD " and resid 50   and name HN  ))
  (( segid "BrD " and resid 49   and name HB  ))
    2.400      2.900      2.100 peak 15021 weight  0.10000E+01 volume  0.11615E+03 ppm1      8.562 ppm2      2.642
OR (15021)
  (( segid "BrD " and resid 46   and name HN  ))
  (( segid "BrD " and resid 44   and name HB2 ))
ASSI (15091)
  (( segid "BrD " and resid 35   and name HN  ))
  (( segid "BrD " and resid 33   and name HB1 ))
    5.000      5.000      0.500 peak 15091 weight  0.10000E+01 volume  0.12753E+02 ppm1      7.735 ppm2      1.073
OR (15091)
  (( segid "BrD " and resid 35   and name HN  ))
  (  segid "BrD " and resid 81   and name HG1%)
ASSI (15181)
  (( segid "BrD " and resid 30   and name HN  ))
  (  segid "BrD " and resid 101  and name HG2%)
    3.900      3.800      1.600 peak 15181 weight  0.10000E+01 volume  0.50580E+02 ppm1     12.275 ppm2      1.601
OR (15181)
  (( segid "BrD " and resid 30   and name HN  ))
  (  segid "BrD " and resid 25   and name HG2%)
ASSI (15221)
  (( segid "BrD " and resid 28   and name HN  ))
  (( segid "BrD " and resid 32   and name HN  ))
    4.200      4.200      1.300 peak 15221 weight  0.10000E+01 volume  0.33692E+02 ppm1      8.166 ppm2      7.752
OR (15221)
  (( segid "BrD " and resid 28   and name HN  ))
  (  segid "BrD " and resid 34   and name HE% )
ASSI (15331)
  (( segid "BrD " and resid 25   and name HN  ))
  (  segid "BrD " and resid 31   and name HB% )
    4.500      4.500      1.000 peak 15331 weight  0.10000E+01 volume  0.22185E+02 ppm1      9.133 ppm2      2.295
OR (15331)
  (( segid "BrD " and resid 25   and name HN  ))
  (( segid "BrD " and resid 22   and name HB2 ))
ASSI (15341)
  (( segid "BrD " and resid 24   and name HN  ))
  (( segid "BrD " and resid 27   and name HN  ))
    3.700      3.400      1.800 peak 15341 weight  0.10000E+01 volume  0.78760E+02 ppm1      8.660 ppm2      8.147
OR (15341)
  (( segid "BrD " and resid 24   and name HN  ))
  (( segid "BrD " and resid 20   and name HN  ))
ASSI (15411)
  (( segid "BrD " and resid 18   and name HN  ))
  (( segid "BrD " and resid 21   and name HG12))
    4.300      4.300      1.200 peak 15411 weight  0.10000E+01 volume  0.29441E+02 ppm1      9.077 ppm2      1.642
OR (15411)
  (( segid "BrD " and resid 18   and name HN  ))
  (  segid "BrD " and resid 63   and name HD1%)
OR (15411)
  (( segid "BrD " and resid 18   and name HN  ))
  (  segid "BrD " and resid 21   and name HG2%)
ASSI (15451)
  (( segid "BrD " and resid 17   and name HN  ))
  (  segid "BrD " and resid 15   and name HD% )
    4.700      4.700      0.800 peak 15451 weight  0.10000E+01 volume  0.16799E+02 ppm1      8.669 ppm2      7.656
OR (15451)
  (( segid "BrD " and resid 17   and name HN  ))
  (  segid "BrD " and resid 106  and name HE% )
ASSI (15461)
  (( segid "BrD " and resid 16   and name HN  ))
  (  segid "BrD " and resid 14   and name HD2%)
    4.800      4.800      0.700 peak 15461 weight  0.10000E+01 volume  0.14734E+02 ppm1      8.791 ppm2      1.430
OR (15461)
  (( segid "BrD " and resid 16   and name HN  ))
  (  segid "BrD " and resid 69   and name HG2%)
OR (15461)
  (( segid "BrD " and resid 16   and name HN  ))
  (  segid "BrD " and resid 14   and name HD1%)
ASSI (15491)
  (( segid "BrD " and resid 14   and name HN  ))
  (( segid "BrD " and resid 15   and name HB1 ))
    5.000      5.000      0.500 peak 15491 weight  0.10000E+01 volume  0.11598E+02 ppm1      8.809 ppm2      3.823
OR (15491)
  (( segid "BrD " and resid 13   and name HN  ))
  (( segid "BrD " and resid 15   and name HB1 ))
ASSI (15501)
  (( segid "BrD " and resid 14   and name HN  ))
  (( segid "BrD " and resid 15   and name HB2 ))
    5.100      5.100      0.400 peak 15501 weight  0.10000E+01 volume  0.11421E+02 ppm1      8.809 ppm2      3.441
OR (15501)
  (( segid "BrD " and resid 13   and name HN  ))
  (( segid "BrD " and resid 15   and name HB2 ))
ASSI (15581)
  (( segid "BrD " and resid 32   and name HE1 ))
  (( segid "BrD " and resid 30   and name HB1 ))
    4.800      4.800      0.700 peak 15581 weight  0.10000E+01 volume  0.15339E+02 ppm1     11.082 ppm2      4.955
OR (15581)
  (( segid "BrD " and resid 32   and name HE1 ))
  (( segid "BrD " and resid 32   and name HA  ))
ASSI (15621)
  (( segid "BrD " and resid 32   and name HE1 ))
  (( segid "BrD " and resid 33   and name HD1 ))
    4.200      4.200      1.300 peak 15621 weight  0.10000E+01 volume  0.36353E+02 ppm1     11.082 ppm2      2.779
OR (15621)
  (( segid "BrD " and resid 32   and name HE1 ))
  (( segid "BrD " and resid 94   and name HB1 ))
ASSI (  862)
  (( segid "BrD " and resid 95   and name HB2 ))
  (( segid "BrD " and resid 95   and name HA  ))
    2.900      2.100      2.100 peak  862 weight  0.10000E+01 volume  0.13207E+03 ppm1      3.373 ppm2      4.477
OR (  862)
  (( segid "BrD " and resid 65   and name HB2 ))
  (( segid "BrD " and resid 62   and name HA  ))
ASSI ( 5972)
  (  segid "BrD " and resid 18   and name HD1%)
  (( segid "BrD " and resid 68   and name HB1 ))
    2.500      2.000      2.000 peak 5972 weight  0.10000E+01 volume  0.16386E+03 ppm1      1.057 ppm2      3.667
OR ( 5972)
  (  segid "BrD " and resid 18   and name HD1%)
  (( segid "BrD " and resid 15   and name HB2 ))
ASSI ( 6172)
  (  segid "BrD " and resid 56   and name HD1%)
  (( segid "BrD " and resid 26   and name HA  ))
    3.000      2.200      2.200 peak 6172 weight  0.10000E+01 volume  0.11879E+03 ppm1      1.546 ppm2      4.502
OR ( 6172)
  (( segid "BrD " and resid 116  and name HG12))
  (( segid "BrD " and resid 75   and name HA  ))
ASSI ( 6592)
  (  segid "BrD " and resid 31   and name HB% )
  (  segid "BrD " and resid 35   and name HE% )
    3.000      2.200      2.200 peak 6592 weight  0.10000E+01 volume  0.12050E+03 ppm1      2.289 ppm2      2.779
OR ( 6592)
  (  segid "BrD " and resid 31   and name HB% )
  (( segid "BrD " and resid 33   and name HD1 ))
ASSI ( 6622)
  (  segid "BrD " and resid 31   and name HB% )
  (( segid "BrD " and resid 56   and name HB2 ))
    3.200      2.600      2.300 peak 6622 weight  0.10000E+01 volume  0.78528E+02 ppm1      2.291 ppm2      1.994
OR ( 6622)
  (  segid "BrD " and resid 31   and name HB% )
  (( segid "BrD " and resid 102  and name HB1 ))
ASSI ( 6812)
  (  segid "BrD " and resid 99   and name HB% )
  (( segid "BrD " and resid 85   and name HB2 ))
    2.500      1.600      1.600 peak 6812 weight  0.10000E+01 volume  0.30669E+03 ppm1      2.190 ppm2      3.645
OR ( 6812)
  (  segid "BrD " and resid 99   and name HB% )
  (( segid "BrD " and resid 82   and name HB1 ))
ASSI ( 6822)
  (  segid "BrD " and resid 99   and name HB% )
  (( segid "BrD " and resid 103  and name HB2 ))
    2.900      2.100      2.100 peak 6822 weight  0.10000E+01 volume  0.12780E+03 ppm1      2.190 ppm2      1.903
OR ( 6822)
  (  segid "BrD " and resid 99   and name HB% )
  (( segid "BrD " and resid 86   and name HG1 ))
ASSI ( 7132)
  (  segid "BrD " and resid 38   and name HG1%)
  (( segid "BrD " and resid 46   and name HB1 ))
    2.600      1.700      1.700 peak 7132 weight  0.10000E+01 volume  0.23427E+03 ppm1      1.057 ppm2      3.306
OR ( 7132)
  (  segid "BrD " and resid 81   and name HG1%)
  (( segid "BrD " and resid 77   and name HB1 ))
ASSI ( 7142)
  (  segid "BrD " and resid 81   and name HG1%)
  (( segid "BrD " and resid 59   and name HB2 ))
    2.800      2.000      2.000 peak 7142 weight  0.10000E+01 volume  0.18258E+03 ppm1      1.058 ppm2      2.475
OR ( 7142)
  (  segid "BrD " and resid 38   and name HG1%)
  (( segid "BrD " and resid 53   and name HG2 ))
ASSI ( 7152)
  (  segid "BrD " and resid 81   and name HG1%)
  (( segid "BrD " and resid 54   and name HB2 ))
    2.800      2.000      2.000 peak 7152 weight  0.10000E+01 volume  0.17360E+03 ppm1      1.057 ppm2      1.962
OR ( 7152)
  (  segid "BrD " and resid 81   and name HG1%)
  (( segid "BrD " and resid 56   and name HB2 ))
ASSI ( 7222)
  (( segid "BrD " and resid 17   and name HB  ))
  (  segid "BrD " and resid 14   and name HD2%)
    3.200      2.600      2.300 peak 7222 weight  0.10000E+01 volume  0.77701E+02 ppm1      4.854 ppm2      1.424
OR ( 7222)
  (( segid "BrD " and resid 17   and name HB  ))
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   (  segid "BrD " and resid 14   and name HD1%)
OR [ 7222]
   (( segid "BrD " and resid 17   and name HB  ))
   (( segid "BrD " and resid 109  and name HG1 ))
ASSI [ 7232]
   (( segid "BrD " and resid 17   and name HB  ))
   (  segid "BrD " and resid 115  and name HD1%)
      3.400      2.900      2.100 peak  7232 weight  0.10000E+01 volume  0.48663E+02 ppm1        4.854 ppm2      1.377
OR [ 7232]
   (( segid "BrD " and resid 17   and name HB  ))
   (  segid "BrD " and resid 14   and name HD2%)
ASSI [ 7262]
   (  segid "BrD " and resid 17   and name HG2%)
   (  segid "BrD " and resid 21   and name HD1%)
      2.400      1.400      1.400 peak  7262 weight  0.10000E+01 volume  0.43712E+03 ppm1        1.747 ppm2      1.221
OR [ 7262]
   (  segid "BrD " and resid 17   and name HG2%)
   (  segid "BrD " and resid 110  and name HG2%)
ASSI [ 7392]
   (( segid "BrD " and resid 15   and name HA  ))
   (( segid "BrD " and resid 18   and name HG  ))
      3.800      3.400      1.700 peak  7392 weight  0.10000E+01 volume  0.25131E+02 ppm1        4.605 ppm2      2.314
OR [ 7392]
   (( segid "BrD " and resid 15   and name HA  ))
   (( segid "BrD " and resid 19   and name HB1 ))
ASSI [ 7742]
   (( segid "BrD " and resid 106  and name HA  ))
   (  segid "BrD " and resid 25   and name HG1%)
      3.400      2.900      2.100 peak  7742 weight  0.10000E+01 volume  0.51959E+02 ppm1        4.557 ppm2      1.817
OR [ 7742]
   (( segid "BrD " and resid 106  and name HA  ))
   (( segid "BrD " and resid 102  and name HB2 ))
ASSI [ 8052]
   (( segid "BrD " and resid 77   and name HB1 ))
   (( segid "BrD " and resid 80   and name HB2 ))
      3.300      2.700      2.200 peak  8052 weight  0.10000E+01 volume  0.59988E+02 ppm1        3.325 ppm2      2.564
OR [ 8052]
   (( segid "BrD " and resid 77   and name HB1 ))
   (( segid "BrD " and resid 54   and name HB1 ))
OR [ 8052]
   (( segid "BrD " and resid 77   and name HB1 ))
   (  segid "BrD " and resid 54   and name HE% )
ASSI [ 8122]
   (( segid "BrD " and resid 63   and name HA  ))
   (( segid "BrD " and resid 62   and name HB1 ))
      3.700      3.400      1.800 peak  8122 weight  0.10000E+01 volume  0.30661E+02 ppm1        5.296 ppm2      2.660
OR [ 8122]
   (( segid "BrD " and resid 63   and name HA  ))
   (( segid "BrD " and resid 67   and name HB2 ))
OR [ 8122]
   (( segid "BrD " and resid 63   and name HA  ))
   (( segid "BrD " and resid 64   and name HB1 ))
ASSI [ 8212]
   (( segid "BrD " and resid 109  and name HG1 ))
   (( segid "BrD " and resid 109  and name HB1 ))
      3.200      1.200      1.200 peak  8212 weight  0.10000E+01 volume  0.72542E+03 ppm1        1.401 ppm2      2.310
OR [ 8212]
   (  segid "BrD " and resid 14   and name HD2%)
   (( segid "BrD " and resid 18   and name HG  ))
ASSI [ 8492]
   (  segid "BrD " and resid 18   and name HD2%)
   (( segid "BrD " and resid 14   and name HA  ))
      2.700      1.800      1.800 peak  8492 weight  0.10000E+01 volume  0.19700E+03 ppm1        0.414 ppm2      4.626
OR [ 8492]
   (  segid "BrD " and resid 18   and name HD2%)
   (( segid "BrD " and resid 15   and name HA  ))
OR [ 8492]
   (  segid "BrD " and resid 18   and name HD2%)
   (( segid "BrD " and resid 71   and name HA  ))
ASSI [ 8542]
   (  segid "BrD " and resid 22   and name HD1%)
   (( segid "BrD " and resid 60   and name HB2 ))
      2.600      1.700      1.700 peak  8542 weight  0.10000E+01 volume  0.24926E+03 ppm1        1.645 ppm2      4.629
OR [ 8542]
   (  segid "BrD " and resid 22   and name HD1%)
   (( segid "BrD " and resid 23   and name HA  ))
OR [ 8542]
   (  segid "BrD " and resid 22   and name HD1%)
   (( segid "BrD " and resid 56   and name HA  ))
OR [ 8542]
   (  segid "BrD " and resid 22   and name HD1%)
   (( segid "BrD " and resid 61   and name HA  ))
ASSI [ 8662]
   (  segid "BrD " and resid 56   and name HD2%)
   (  segid "BrD " and resid 22   and name HD2%)
      2.200      1.200      1.200 peak  8662 weight  0.10000E+01 volume  0.65442E+03 ppm1        1.254 ppm2      1.635
OR [ 8662]
   (  segid "BrD " and resid 56   and name HD2%)
   (  segid "BrD " and resid 25   and name HG2%)
ASSI [ 8712]
   (  segid "BrD " and resid 56   and name HD1%)
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   (  segid "BrD " and resid 102  and name HD1%)
      2.600      1.700      1.700 peak  8712 weight  0.10000E+01 volume  0.26563E+03 ppm1        1.567 ppm2      1.321
OR [ 8712]
   (  segid "BrD " and resid 56   and name HD1%)
   (  segid "BrD " and resid 102  and name HD2%)
OR [ 8712]
   (( segid "BrD " and resid 116  and name HG12))
   (  segid "BrD " and resid 115  and name HD1%)
ASSI [ 8962]
   (( segid "BrD " and resid 56   and name HB2 ))
   (  segid "BrD " and resid 25   and name HG2%)
      3.700      3.400      1.800 peak  8962 weight  0.10000E+01 volume  0.31139E+02 ppm1        1.994 ppm2      1.627
OR [ 8962]
   (( segid "BrD " and resid 102  and name HB1 ))
   (  segid "BrD " and resid 101  and name HG2%)
OR [ 8962]
   (( segid "BrD " and resid 56   and name HB2 ))
   (  segid "BrD " and resid 22   and name HD2%)
ASSI [ 9112]
   (  segid "BrD " and resid 21   and name HG2%)
   (  segid "BrD " and resid 102  and name HD2%)
      2.600      1.700      1.700 peak  9112 weight  0.10000E+01 volume  0.28598E+03 ppm1        1.600 ppm2      1.324
OR [ 9112]
   (  segid "BrD " and resid 101  and name HG2%)
   (  segid "BrD " and resid 102  and name HD1%)
ASSI [ 9142]
   (  segid "BrD " and resid 21   and name HG2%)
   (  segid "BrD " and resid 78   and name HD1%)
      3.800      3.600      1.700 peak  9142 weight  0.10000E+01 volume  0.27968E+02 ppm1        1.896 ppm2      0.773
OR [ 9142]
   (  segid "BrD " and resid 21   and name HG2%)
   (  segid "BrD " and resid 81   and name HG2%)
ASSI [ 9192]
   (  segid "BrD " and resid 21   and name HD1%)
   (  segid "BrD " and resid 18   and name HD1%)
      2.500      1.600      1.600 peak  9192 weight  0.10000E+01 volume  0.36076E+03 ppm1        1.205 ppm2      1.068
OR [ 9192]
   (  segid "BrD " and resid 21   and name HD1%)
   (( segid "BrD " and resid 78   and name HB2 ))
ASSI [ 9662]
   (( segid "BrD " and resid 79   and name HG1 ))
   (  segid "BrD " and resid 83   and name HG2%)
      3.000      2.200      2.200 peak  9662 weight  0.10000E+01 volume  0.10300E+03 ppm1        3.031 ppm2      1.900
OR [ 9662]
   (( segid "BrD " and resid 79   and name HG1 ))
   (( segid "BrD " and resid 116  and name HG11))
ASSI [10002]
   (( segid "BrD " and resid 54   and name HB1 ))
   (  segid "BrD " and resid 81   and name HG1%)
      3.600      3.200      1.900 peak 10002 weight  0.10000E+01 volume  0.33897E+02 ppm1        2.585 ppm2      1.083
OR [10002]
   (( segid "BrD " and resid 42   and name HB2 ))
   (  segid "BrD " and resid 38   and name HG1%)
ASSI [10092]
   (( segid "BrD " and resid 35   and name HG1 ))
   (( segid "BrD " and resid 32   and name HA  ))
      3.100      2.400      2.400 peak 10092 weight  0.10000E+01 volume  0.97444E+02 ppm1        3.422 ppm2      4.972
OR [10092]
   (( segid "BrD " and resid 35   and name HG1 ))
   (( segid "BrD " and resid 31   and name HA  ))
ASSI [10182]
   (( segid "BrD " and resid 52   and name HB1 ))
   (( segid "BrD " and resid 80   and name HG1 ))
      4.100      4.100      1.400 peak 10182 weight  0.10000E+01 volume  0.17926E+02 ppm1        3.621 ppm2      2.345
OR [10182]
   (( segid "BrD " and resid 84   and name HB1 ))
   (( segid "BrD " and resid 80   and name HG1 ))
ASSI [10302]
   (( segid "BrD " and resid 42   and name HG1 ))
   (( segid "BrD " and resid 39   and name HD1 ))
      3.000      2.200      2.200 peak 10302 weight  0.10000E+01 volume  0.10808E+03 ppm1        2.880 ppm2      2.298
OR [10302]
   (( segid "BrD " and resid 7    and name HG1 ))
   (( segid "BrD " and resid 6    and name HB2 ))
ASSI [10412]
   (( segid "BrD " and resid 48   and name HA  ))
   (( segid "BrD " and resid 48   and name HB1 ))
      2.800      2.000      2.000 peak 10412 weight  0.10000E+01 volume  0.17461E+03 ppm1        4.831 ppm2      2.762
OR [10412]
   (( segid "BrD " and resid 87   and name HA  ))
   (( segid "BrD " and resid 87   and name HB1 ))
ASSI [10502]
   (( segid "BrD " and resid 112  and name HB1 ))
   (  segid "BrD " and resid 113  and name HB% )
      2.700      1.800      1.800 peak 10502 weight  0.10000E+01 volume  0.19681E+03 ppm1        2.684 ppm2      1.985
OR [10502]
   (( segid "BrD " and resid 112  and name HB1 ))
   (( segid "BrD " and resid 109  and name HD1 ))
ASSI [10602]
   (( segid "BrD " and resid 23   and name HA  ))
   (( segid "BrD " and resid 19   and name HA  ))
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    3.500      3.100      2.000 peak 10602 weight  0.10000E+01 volume  0.44566E+02 ppm1      4.656 ppm2      4.278
OR (10602)
  (( segid "BrD " and resid 104   and name HA  ))
  (( segid "BrD " and resid 101   and name HA  ))
ASSI (10902)
  (( segid "BrD " and resid 70    and name HB1 ))
  (( segid "BrD " and resid 11    and name HG1 ))
    3.200      2.600      2.300 peak 10902 weight  0.10000E+01 volume  0.71093E+02 ppm1      4.755 ppm2      2.646
OR (10902)
  (( segid "BrD " and resid 70    and name HB1 ))
  (  segid "BrD " and resid 75    and name HE% )
OR (10902)
  (( segid "BrD " and resid 93    and name HB2 ))
  (( segid "BrD " and resid 97    and name HB1 ))
OR (10902)
  (( segid "BrD " and resid 70    and name HB1 ))
  (( segid "BrD " and resid 62    and name HB1 ))
OR (10902)
  (( segid "BrD " and resid 70    and name HB1 ))
  (( segid "BrD " and resid 8     and name HG1 ))
ASSI (11592)
  (( segid "BrD " and resid 109   and name HB2 ))
  (  segid "BrD " and resid 21    and name HD1%)
    3.400      2.900      2.100 peak 11592 weight  0.10000E+01 volume  0.47549E+02 ppm1      2.141 ppm2      1.232
OR (11592)
  (( segid "BrD " and resid 109   and name HB2 ))
  (  segid "BrD " and resid 110   and name HG2%)
ASSI (11652)
  (( segid "BrD " and resid 59    and name HB2 ))
  (  segid "BrD " and resid 58    and name HG2%)
    2.900      2.100      2.100 peak 11652 weight  0.10000E+01 volume  0.12259E+03 ppm1      2.487 ppm2      1.660
OR (11652)
  (( segid "BrD " and resid 59    and name HB2 ))
  (  segid "BrD " and resid 22    and name HD1%)
ASSI (12162)
  (( segid "BrD " and resid 18    and name HA  ))
  (  segid "BrD " and resid 21    and name HG2%)
    3.600      3.200      1.900 peak 12162 weight  0.10000E+01 volume  0.38701E+02 ppm1      3.866 ppm2      1.591
OR (12162)
  (( segid "BrD " and resid 18    and name HA  ))
  (  segid "BrD " and resid 22    and name HD2%)
ASSI (12172)
  (( segid "BrD " and resid 6     and name HA  ))
  (( segid "BrD " and resid 6     and name HG2 ))
    2.500      1.600      1.600 peak 12172 weight  0.10000E+01 volume  0.31535E+03 ppm1      4.951 ppm2      2.033
OR (12172)
  (( segid "BrD " and resid 39    and name HA  ))
  (( segid "BrD " and resid 39    and name HG1 ))
ASSI (12302)
  (( segid "BrD " and resid 86    and name HG2 ))
  (( segid "BrD " and resid 81    and name HA  ))
    3.600      3.200      1.900 peak 12302 weight  0.10000E+01 volume  0.36612E+02 ppm1      0.740 ppm2      4.450
OR (12302)
  (( segid "BrD " and resid 86    and name HG2 ))
  (( segid "BrD " and resid 96    and name HA  ))
ASSI (12572)
  (  segid "BrD " and resid 59    and name HE% )
  (  segid "BrD " and resid 22    and name HD1%)
    2.700      1.800      1.800 peak 12572 weight  0.10000E+01 volume  0.19213E+03 ppm1      1.848 ppm2      1.645
OR (12572)
  (  segid "BrD " and resid 59    and name HE% )
  (  segid "BrD " and resid 63    and name HD1%)
ASSI (12722)
  (  segid "BrD " and resid 18    and name HD1%)
  (( segid "BrD " and resid 68    and name HB2 ))
    3.400      2.900      2.100 peak 12722 weight  0.10000E+01 volume  0.56232E+02 ppm1      1.056 ppm2      3.513
OR (12722)
  (  segid "BrD " and resid 18    and name HD1%)
  (( segid "BrD " and resid 75    and name HG1 ))
ASSI (12742)
  (( segid "BrD " and resid 72    and name HA  ))
  (  segid "BrD " and resid 116   and name HG2%)
    3.000      2.200      2.200 peak 12742 weight  0.10000E+01 volume  0.10372E+03 ppm1      4.656 ppm2      1.414
OR (12742)
  (( segid "BrD " and resid 67    and name HA  ))
  (  segid "BrD " and resid 69    and name HG2%)
OR (12742)
  (( segid "BrD " and resid 111   and name HA  ))
  (  segid "BrD " and resid 116   and name HD1%)
ASSI (12862)
  (( segid "BrD " and resid 62    and name HD1 ))
  (  segid "BrD " and resid 54    and name HE% )
    3.000      2.200      2.200 peak 12862 weight  0.10000E+01 volume  0.10219E+03 ppm1      3.177 ppm2      2.569
OR (12862)
  (( segid "BrD " and resid 62    and name HD1 ))
  (( segid "BrD " and resid 63    and name HB2 ))
OR (12862)
  (( segid "BrD " and resid 62    and name HD1 ))
  (( segid "BrD " and resid 54    and name HB1 ))
ASSI (13242)
  (( segid "BrD " and resid 46    and name HB2 ))
  (  segid "BrD " and resid 38    and name HG2%)
    3.500      3.100      2.000 peak 13242 weight  0.10000E+01 volume  0.46826E+02 ppm1      3.080 ppm2      0.791
OR (13242)
  (( segid "BrD " and resid 46    and name HB2 ))
  (( segid "BrD " and resid 50    and name HG12))
ASSI (13322)
  (  segid "BrD " and resid 78    and name HD2%)
  (  segid "BrD " and resid 21    and name HD2%)
    2.700      1.800      1.800 peak 13322 weight  0.10000E+01 volume  0.21424E+03 ppm1      0.662 ppm2      1.590
OR (13322)
  (  segid "BrD " and resid 78    and name HD2%)
  (  segid "BrD " and resid 22    and name HD2%)
ASSI (13352)
  (  segid "BrD " and resid 18    and name HD2%)
  (( segid "BrD " and resid 14    and name HB1 ))
    4.200      4.200      1.300 peak 13352 weight  0.10000E+01 volume  0.14748E+02 ppm1      0.415 ppm2      2.481
OR (13352)
  (  segid "BrD " and resid 18    and name HD2%)
  (( segid "BrD " and resid 21    and name HB  ))
ASSI (13392)
  (  segid "BrD " and resid 25    and name HG1%)
  (( segid "BrD " and resid 26    and name HA  ))
    2.800      2.000      2.000 peak 13392 weight  0.10000E+01 volume  0.16152E+03 ppm1      1.795 ppm2      4.566
OR (13392)
  (  segid "BrD " and resid 25    and name HG1%)
  (( segid "BrD " and resid 106   and name HA  ))
ASSI (13592)
  (  segid "BrD " and resid 56    and name HD2%)
  (( segid "BrD " and resid 59    and name HB2 ))
    2.600      1.700      1.700 peak 13592 weight  0.10000E+01 volume  0.24679E+03 ppm1      1.254 ppm2      2.499
OR (13592)
  (  segid "BrD " and resid 56    and name HD2%)
  (  segid "BrD " and resid 54    and name HE% )
OR (13592)
  (  segid "BrD " and resid 56    and name HD2%)
  (( segid "BrD " and resid 26    and name HB1 ))
ASSI (13602)
  (  segid "BrD " and resid 54    and name HE% )
  (( segid "BrD " and resid 37    and name HB2 ))
    2.500      1.600      1.600 peak 13602 weight  0.10000E+01 volume  0.34655E+03 ppm1      2.535 ppm2      2.323
OR (13602)
  (  segid "BrD " and resid 54    and name HE% )
  (( segid "BrD " and resid 56    and name HG  ))
ASSI (13762)
  (  segid "BrD " and resid 63    and name HD2%)
  (( segid "BrD " and resid 19    and name HB1 ))
    2.300      1.300      1.300 peak 13762 weight  0.10000E+01 volume  0.59623E+03 ppm1      1.498 ppm2      2.318
OR (13762)
  (  segid "BrD " and resid 63    and name HD2%)
  (( segid "BrD " and resid 22    and name HB2 ))
ASSI (13952)
  (  segid "BrD " and resid 14    and name HD1%)
  (( segid "BrD " and resid 14    and name HA  ))
    2.700      1.800      1.800 peak 13952 weight  0.10000E+01 volume  0.20695E+03 ppm1      1.402 ppm2      4.687
OR (13952)
  (  segid "BrD " and resid 14    and name HD1%)
  (( segid "BrD " and resid 69    and name HA  ))
ASSI (14042)
  (  segid "BrD " and resid 76    and name HB% )
  (  segid "BrD " and resid 73    and name HD1%)
    3.100      2.400      2.400 peak 14042 weight  0.10000E+01 volume  0.97985E+02 ppm1      2.092 ppm2      1.540
OR (14042)
  (  segid "BrD " and resid 76    and name HB% )
  (( segid "BrD " and resid 116   and name HG12))
ASSI (14162)
  (( segid "BrD " and resid 15    and name HA  ))
  (  segid "BrD " and resid 63    and name HD2%)
    3.600      3.200      1.900 peak 14162 weight  0.10000E+01 volume  0.37938E+02 ppm1      4.609 ppm2      1.490
OR (14162)
  (( segid "BrD " and resid 60    and name HB2 ))
  (  segid "BrD " and resid 63    and name HD2%)
ASSI (14192)
  (( segid "BrD " and resid 62    and name HA  ))
  (( segid "BrD " and resid 68    and name HB2 ))
    3.700      3.400      1.800 peak 14192 weight  0.10000E+01 volume  0.29812E+02 ppm1      4.459 ppm2      3.504
OR (14192)
  (( segid "BrD " and resid 95    and name HA  ))
  (( segid "BrD " and resid 89    and name HB2 ))
ASSI (14202)
  (( segid "BrD " and resid 95    and name HA  ))
  (( segid "BrD " and resid 98    and name HB2 ))
    3.200      2.600      2.300 peak 14202 weight  0.10000E+01 volume  0.81269E+02 ppm1      4.462 ppm2      3.701
OR (14202)
  (( segid "BrD " and resid 62    and name HA  ))
  (( segid "BrD " and resid 68    and name HB1 ))
ASSI (14312)
  (  segid "BrD " and resid 22    and name HD2%)
  (( segid "BrD " and resid 59    and name HB2 ))
    2.700      1.800      1.800 peak 14312 weight  0.10000E+01 volume  0.21510E+03 ppm1      1.599 ppm2      2.501
OR (14312)
  (  segid "BrD " and resid 22    and name HD2%)
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   (( segid "BrD " and resid 21   and name HB  ))
OR (14312)
   (  segid "BrD " and resid 22   and name HD2%)
   (( segid "BrD " and resid 63   and name HB2 ))
OR (14312)
   (  segid "BrD " and resid 22   and name HD2%)
   (( segid "BrD " and resid 26   and name HB1 ))
ASSI (14432)
   (  segid "BrD " and resid 21   and name HD1%)
   (( segid "BrD " and resid 18   and name HB1 ))
      2.700      1.800      1.800 peak 14432 weight  0.10000E+01 volume  0.19246E+03 ppm1      1.205 ppm2      2.148
OR (14432)
   (  segid "BrD " and resid 21   and name HD1%)
   (( segid "BrD " and resid 102  and name HG  ))
ASSI (14462)
   (  segid "BrD " and resid 110  and name HD1%)
   (  segid "BrD " and resid 116  and name HD1%)
      2.100      1.100      1.100 peak 14462 weight  0.10000E+01 volume  0.89267E+03 ppm1      1.154 ppm2      1.387
OR (14462)
   (  segid "BrD " and resid 110  and name HD1%)
   (  segid "BrD " and resid 115  and name HD1%)
ASSI (14602)
   (  segid "BrD " and resid 18   and name HD1%)
   (  segid "BrD " and resid 115  and name HD1%)
      3.500      3.100      2.000 peak 14602 weight  0.10000E+01 volume  0.42578E+02 ppm1      1.057 ppm2      1.327
OR (14602)
   (  segid "BrD " and resid 18   and name HD1%)
   (( segid "BrD " and resid 78   and name HB1 ))
ASSI (14642)
   (( segid "BrD " and resid 18   and name HA  ))
   (  segid "BrD " and resid 102  and name HD2%)
      4.400      4.400      1.100 peak 14642 weight  0.10000E+01 volume  0.11486E+02 ppm1      3.867 ppm2      1.320
OR (14642)
   (( segid "BrD " and resid 18   and name HA  ))
   (  segid "BrD " and resid 115  and name HD1%)
OR (14642)
   (( segid "BrD " and resid 18   and name HA  ))
   (( segid "BrD " and resid 78   and name HB1 ))
ASSI (14682)
   (  segid "BrD " and resid 22   and name HD1%)
   (( segid "BrD " and resid 64   and name HG1 ))
      3.000      2.200      2.200 peak 14682 weight  0.10000E+01 volume  0.10496E+03 ppm1      1.645 ppm2      2.186
OR (14682)
   (( segid "BrD " and resid 110  and name HG12))
   (( segid "BrD " and resid 115  and name HB1 ))
ASSI (14692)
   (  segid "BrD " and resid 63   and name HD2%)
   (( segid "BrD " and resid 19   and name HD1 ))
      2.300      1.300      1.300 peak 14692 weight  0.10000E+01 volume  0.59246E+03 ppm1      1.498 ppm2      2.191
OR (14692)
   (  segid "BrD " and resid 63   and name HD2%)
   (( segid "BrD " and resid 64   and name HG1 ))
ASSI (14792)
   (  segid "BrD " and resid 22   and name HD2%)
   (( segid "BrD " and resid 56   and name HA  ))
      2.600      1.700      1.700 peak 14792 weight  0.10000E+01 volume  0.26795E+03 ppm1      1.599 ppm2      4.619
OR (14792)
   (  segid "BrD " and resid 32   and name HD2%)
   (( segid "BrD " and resid 60   and name HB2 ))
ASSI (14802)
   (( segid "BrD " and resid 86   and name HD1 ))
   (( segid "BrD " and resid 83   and name HA  ))
      2.700      1.800      1.800 peak 14802 weight  0.10000E+01 volume  0.19483E+03 ppm1      1.896 ppm2      4.461
OR (14802)
   (( segid "BrD " and resid 103  and name HB2 ))
   (( segid "BrD " and resid 99   and name HA  ))
ASSI (14862)
   (( segid "BrD " and resid 54   and name HA  ))
   (  segid "BrD " and resid 81   and name HG1%)
      3.800      3.600      1.700 peak 14862 weight  0.10000E+01 volume  0.25126E+02 ppm1      5.543 ppm2      1.076
OR (14862)
   (( segid "BrD " and resid 54   and name HA  ))
   (  segid "BrD " and resid 38   and name HG1%)
ASSI (14872)
   (  segid "BrD " and resid 81   and name HG1%)
   (( segid "BrD " and resid 80   and name HB2 ))
      2.900      2.100      2.100 peak 14872 weight  0.10000E+01 volume  0.14378E+03 ppm1      1.058 ppm2      2.565
OR (14872)
   (  segid "BrD " and resid 81   and name HG1%)
   (( segid "BrD " and resid 80   and name HB1 ))
OR (14872)
   (  segid "BrD " and resid 81   and name HG1%)
   (  segid "BrD " and resid 54   and name HE% )
OR (14872)
   (  segid "BrD " and resid 81   and name HG1%)
   (( segid "BrD " and resid 54   and name HB1 ))
ASSI (14882)
   (  segid "BrD " and resid 81   and name HG1%)
   (( segid "BrD " and resid 56   and name HG  ))
      3.500      3.100      2.000 peak 14882 weight  0.10000E+01 volume  0.44935E+02 ppm1      1.058 ppm2      2.328
OR (14882)
   (  segid "BrD " and resid 38   and name HG1%)
   (( segid "BrD " and resid 37   and name HB2 ))
ASSI (15202)
   (( segid "BrD " and resid 72   and name HA  ))
   (( segid "BrD " and resid 75   and name HG2 ))
      4.000      4.000      1.500 peak 15202 weight  0.10000E+01 volume  0.18586E+02 ppm1      4.656 ppm2      3.224
OR (15202)
   (( segid "BrD " and resid 61   and name HA  ))
   (( segid "BrD " and resid 59   and name HG2 ))
OR (15202)
   (( segid "BrD " and resid 61   and name HA  ))
   (( segid "BrD " and resid 59   and name HG1 ))
ASSI (15382)
   (( segid "BrD " and resid 74   and name HA  ))
   (  segid "BrD " and resid 75   and name HE% )
      3.200      2.600      2.300 peak 15382 weight  0.10000E+01 volume  0.70547E+02 ppm1      4.362 ppm2      2.653
OR (15382)
   (( segid "BrD " and resid 74   and name HA  ))
   (( segid "BrD " and resid 59   and name HB1 ))
ASSI (15392)
   (( segid "BrD " and resid 74   and name HB1 ))
   (( segid "BrD " and resid 73   and name HB2 ))
      3.200      2.600      2.300 peak 15392 weight  0.10000E+01 volume  0.74692E+02 ppm1      3.572 ppm2      2.471
OR (15392)
   (( segid "BrD " and resid 74   and name HB1 ))
   (( segid "BrD " and resid 63   and name HG  ))
ASSI (15532)
   (( segid "BrD " and resid 82   and name HB2 ))
   (( segid "BrD " and resid 103  and name HB1 ))
      3.100      2.400      2.400 peak 15532 weight  0.10000E+01 volume  0.91806E+02 ppm1      3.573 ppm2      2.344
OR (15532)
   (( segid "BrD " and resid 82   and name HB2 ))
   (( segid "BrD " and resid 86   and name HB1 ))
ASSI (15542)
   (( segid "BrD " and resid 82   and name HB1 ))
   (( segid "BrD " and resid 103  and name HB1 ))
      3.100      2.400      2.400 peak 15542 weight  0.10000E+01 volume  0.94295E+02 ppm1      3.672 ppm2      2.344
OR (15542)
   (( segid "BrD " and resid 107  and name HB1 ))
   (( segid "BrD " and resid 110  and name HB  ))
OR (15542)
   (( segid "BrD " and resid 107  and name HB1 ))
   (( segid "BrD " and resid 103  and name HB1 ))
OR (15542)
   (( segid "BrD " and resid 106  and name HB2 ))
   (( segid "BrD " and resid 109  and name HB1 ))
OR (15542)
   (( segid "BrD " and resid 106  and name HB2 ))
   (( segid "BrD " and resid 21   and name HG11))
ASSI (15562)
   (( segid "BrD " and resid 82   and name HB1 ))
   (( segid "BrD " and resid 103  and name HB2 ))
      3.500      3.100      2.000 peak 15562 weight  0.10000E+01 volume  0.43748E+02 ppm1      3.671 ppm2      1.897
OR (15562)
   (( segid "BrD " and resid 82   and name HB1 ))
   (  segid "BrD " and resid 83   and name HG2%)
ASSI (15572)
   (( segid "BrD " and resid 106  and name HB2 ))
   (( segid "BrD " and resid 110  and name HG11))
      5.500      5.500      0.000 peak 15572 weight  0.10000E+01 volume  0.17071E+01 ppm1      3.671 ppm2      1.722
OR (15572)
   (( segid "BrD " and resid 107  and name HB1 ))
   (( segid "BrD " and resid 110  and name HG11))
OR (15572)
   (( segid "BrD " and resid 106  and name HB2 ))
   (  segid "BrD " and resid 17   and name HG2%)
ASSI (15582)
   (( segid "BrD " and resid 15   and name HB2 ))
   (  segid "BrD " and resid 63   and name HD1%)
      3.300      2.700      2.200 peak 15582 weight  0.10000E+01 volume  0.63482E+02 ppm1      3.671 ppm2      1.653
OR (15582)
   (( segid "BrD " and resid 106  and name HB2 ))
   (( segid "BrD " and resid 110  and name HG12))
OR (15582)
   (( segid "BrD " and resid 107  and name HB1 ))
   (( segid "BrD " and resid 110  and name HG12))
ASSI (15722)
   (( segid "BrD " and resid 52   and name HB1 ))
   (( segid "BrD " and resid 80   and name HB1 ))
      4.700      4.700      0.800 peak 15722 weight  0.10000E+01 volume  0.74610E+01 ppm1      3.620 ppm2      2.597
OR (15722)
   (( segid "BrD " and resid 84   and name HB1 ))
   (( segid "BrD " and resid 87   and name HB2 ))
OR (15722)
   (( segid "BrD " and resid 84   and name HB1 ))
   (( segid "BrD " and resid 80   and name HB1 ))
OR (15722)
   (( segid "BrD " and resid 65   and name HB1 ))
   (( segid "BrD " and resid 64   and name HB1 ))
ASSI (16012)
   (( segid "BrD " and resid 68   and name HA  ))
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   ( segid "BrD " and resid 69   and name HG2%)
     3.700      3.400      1.800 peak 16012 weight  0.10000E+01 volume  0.30406E+02 ppm1      5.148 ppm2      1.433
OR (16012)
   (( segid "BrD " and resid 68   and name HA  ))
   ( segid "BrD " and resid 14   and name HD2%)
ASSI (16172)
   (( segid "BrD " and resid 68   and name HB1 ))
   ( segid "BrD " and resid 63   and name HD1%)
     3.600      3.200      1.900 peak 16172 weight  0.10000E+01 volume  0.37293E+02 ppm1      3.668 ppm2      1.645
OR (16172)
   (( segid "BrD " and resid 68   and name HB1 ))
   ( segid "BrD " and resid 22   and name HD1%)
ASSI (16182)
   (( segid "BrD " and resid 68   and name HB2 ))
   ( segid "BrD " and resid 63   and name HD1%)
     3.800      3.600      1.700 peak 16182 weight  0.10000E+01 volume  0.27740E+02 ppm1      3.522 ppm2      1.645
OR (16182)
   (( segid "BrD " and resid 68   and name HB2 ))
   ( segid "BrD " and resid 22   and name HD1%)
ASSI (16362)
   (( segid "BrD " and resid 97   and name HE1 ))
   ( segid "BrD " and resid 101  and name HD1%)
     3.000      2.200      2.300 peak 16362 weight  0.10000E+01 volume  0.11543E+03 ppm1      3.571 ppm2      1.580
OR (16362)
   (( segid "BrD " and resid 64   and name HE1 ))
   ( segid "BrD " and resid 22   and name HD2%)
OR (16362)
   (( segid "BrD " and resid 97   and name HE1 ))
   ( segid "BrD " and resid 101  and name HG2%)
ASSI (16372)
   (( segid "BrD " and resid 88   and name HB1 ))
   (( segid "BrD " and resid 50   and name HG11))
     2.900      2.100      2.100 peak 16372 weight  0.10000E+01 volume  0.13106E+03 ppm1      3.522 ppm2      1.401
OR (16372)
   (( segid "BrD " and resid 111  and name HE1 ))
   ( segid "BrD " and resid 116  and name HD1%)
ASSI (16482)
   (( segid "BrD " and resid 96   and name HA  ))
   (( segid "BrD " and resid 85   and name HB1 ))
     3.800      3.600      1.700 peak 16482 weight  0.10000E+01 volume  0.24633E+02 ppm1      4.409 ppm2      3.891
OR (16482)
   (( segid "BrD " and resid 107  and name HA  ))
   (( segid "BrD " and resid 106  and name HB1 ))
ASSI (16572)
   (( segid "BrD " and resid 96   and name HB2 ))
   (( segid "BrD " and resid 86   and name HA  ))
     4.100      4.100      1.400 peak 16572 weight  0.10000E+01 volume  0.16756E+02 ppm1      3.132 ppm2      4.804
OR (16572)
   (( segid "BrD " and resid 96   and name HB2 ))
   (( segid "BrD " and resid 92   and name HA  ))
ASSI (16582)
   (( segid "BrD " and resid 96   and name HB1 ))
   (( segid "BrD " and resid 92   and name HA  ))
     3.800      3.600      1.700 peak 16582 weight  0.10000E+01 volume  0.28094E+02 ppm1      4.004 ppm2      4.808
OR (16582)
   (( segid "BrD " and resid 96   and name HB1 ))
   (( segid "BrD " and resid 97   and name HA  ))
OR (16582)
   (( segid "BrD " and resid 96   and name HB1 ))
   (( segid "BrD " and resid 94   and name HA  ))
ASSI (16782)
   (( segid "BrD " and resid 95   and name HB1 ))
   (( segid "BrD " and resid 85   and name HA  ))
     3.200      2.600      2.300 peak 16782 weight  0.10000E+01 volume  0.73175E+02 ppm1      3.620 ppm2      4.995
OR (16782)
   (( segid "BrD " and resid 95   and name HB1 ))
   (( segid "BrD " and resid 93   and name HB1 ))
OR (16782)
   (( segid "BrD " and resid 84   and name HB1 ))
   (( segid "BrD " and resid 85   and name HA  ))
ASSI (16852)
   (( segid "BrD " and resid 82   and name HB1 ))
   ( segid "BrD " and resid 107  and name HE% )
     3.000      2.200      2.200 peak 16852 weight  0.10000E+01 volume  0.10660E+03 ppm1      3.670 ppm2      7.696
OR (16852)
   (( segid "BrD " and resid 107  and name HB1 ))
   ( segid "BrD " and resid 107  and name HE% )
ASSI (17112)
   (( segid "BrD " and resid 95   and name HB2 ))
   (( segid "BrD " and resid 32   and name HH2 ))
     3.500      3.100      2.000 peak 17112 weight  0.10000E+01 volume  0.46090E+02 ppm1      3.366 ppm2      7.754
OR (17112)
   (( segid "BrD " and resid 95   and name HB2 ))
   ( segid "BrD " and resid 34   and name HE% )
OR (17112)
   (( segid "BrD " and resid 95   and name HB2 ))
   ( segid "BrD " and resid 96   and name HD% )
ASSI (17122)
   (( segid "BrD " and resid 105  and name HB1 ))
   ( segid "BrD " and resid 25   and name HG1%)
     3.400      2.900      2.100 peak 17122 weight  0.10000E+01 volume  0.47791E+02 ppm1      3.721 ppm2      1.824
OR (17122)
   (( segid "BrD " and resid 105  and name HB1 ))
   (( segid "BrD " and resid 102  and name HB2 ))
ASSI (17132)
   (( segid "BrD " and resid 106  and name HB2 ))
   (( segid "BrD " and resid 102  and name HB2 ))
     3.500      3.100      2.000 peak 17132 weight  0.10000E+01 volume  0.42104E+02 ppm1      3.668 ppm2      1.824
OR (17132)
   (( segid "BrD " and resid 105  and name HB2 ))
   ( segid "BrD " and resid 25   and name HG1%)
OR (17132)
   (( segid "BrD " and resid 106  and name HB2 ))
   ( segid "BrD " and resid 25   and name HG1%)
ASSI (17142)
   (( segid "BrD " and resid 106  and name HB2 ))
   ( segid "BrD " and resid 21   and name HG2%)
     3.700      3.400      1.800 peak 17142 weight  0.10000E+01 volume  0.28702E+02 ppm1      3.668 ppm2      1.612
OR (17142)
   (( segid "BrD " and resid 105  and name HB2 ))
   ( segid "BrD " and resid 101  and name HG2%)
OR (17142)
   (( segid "BrD " and resid 105  and name HB2 ))
   ( segid "BrD " and resid 21   and name HG2%)
ASSI (17272)
   (( segid "BrD " and resid 116  and name HA  ))
   ( segid "BrD " and resid 110  and name HG2%)
     4.000      4.000      1.500 peak 17272 weight  0.10000E+01 volume  0.18200E+02 ppm1      4.804 ppm2      1.262
OR (17272)
   (( segid "BrD " and resid 57   and name HA  ))
   ( segid "BrD " and resid 56   and name HD2%)
ASSI (17322)
   (( segid "BrD " and resid 59   and name HA  ))
   (( segid "BrD " and resid 62   and name HG2 ))
     4.200      4.200      1.300 peak 17322 weight  0.10000E+01 volume  0.13830E+02 ppm1      4.903 ppm2      1.490
OR (17322)
   (( segid "BrD " and resid 20   and name HA  ))
   ( segid "BrD " and resid 63   and name HD2%)
ASSI (17492)
   (( segid "BrD " and resid 34   and name HA  ))
   (( segid "BrD " and resid 31   and name HA  ))
     3.300      2.700      2.200 peak 17492 weight  0.10000E+01 volume  0.57702E+02 ppm1      5.544 ppm2      4.989
OR (17492)
   (( segid "BrD " and resid 34   and name HA  ))
   (( segid "BrD " and resid 32   and name HA  ))
ASSI (17522)
   (( segid "BrD " and resid 34   and name HA  ))
   ( segid "BrD " and resid 54   and name HE% )
     4.000      4.000      1.500 peak 17522 weight  0.10000E+01 volume  0.19574E+02 ppm1      5.544 ppm2      2.564
OR (17522)
   (( segid "BrD " and resid 34   and name HA  ))
   (( segid "BrD " and resid 37   and name HG2 ))
ASSI (17682)
   (( segid "BrD " and resid 33   and name HG1 ))
   (( segid "BrD " and resid 32   and name HE3 ))
     4.900      4.900      0.600 peak 17682 weight  0.10000E+01 volume  0.54467E+01 ppm1      0.859 ppm2      7.926
OR (17682)
   (( segid "BrD " and resid 33   and name HG1 ))
   (( segid "BrD " and resid 34   and name HZ  ))
ASSI (17692)
   (( segid "BrD " and resid 33   and name HG1 ))
   (( segid "BrD " and resid 32   and name HE3 ))
     4.000      4.000      1.500 peak 17692 weight  0.10000E+01 volume  0.18980E+02 ppm1      0.859 ppm2      7.803
OR (17692)
   (( segid "BrD " and resid 33   and name HG1 ))
   ( segid "BrD " and resid 34   and name HE% )
ASSI (17702)
   (( segid "BrD " and resid 33   and name HG1 ))
   (( segid "BrD " and resid 32   and name HH2 ))
     4.100      4.100      1.400 peak 17702 weight  0.10000E+01 volume  0.16294E+02 ppm1      0.859 ppm2      7.745
OR (17702)
   (( segid "BrD " and resid 33   and name HG1 ))
   ( segid "BrD " and resid 34   and name HE% )
ASSI (17892)
   (( segid "BrD " and resid 33   and name HD1 ))
   ( segid "BrD " and resid 34   and name HD% )
     3.400      2.900      2.100 peak 17892 weight  0.10000E+01 volume  0.51743E+02 ppm1      2.783 ppm2      7.720
OR (17892)
   (( segid "BrD " and resid 33   and name HD1 ))
   (( segid "BrD " and resid 32   and name HH2 ))
ASSI (17972)
   (( segid "BrD " and resid 33   and name HB2 ))
   (( segid "BrD " and resid 32   and name HZ3 ))
     3.500      3.100      2.000 peak 17972 weight  0.10000E+01 volume  0.44678E+02 ppm1     -0.176 ppm2      7.789
OR (17972)
   (( segid "BrD " and resid 33   and name HB2 ))
   ( segid "BrD " and resid 34   and name HE% )
ASSI (18022)
   (( segid "BrD " and resid 59   and name HG2 ))
   (( segid "BrD " and resid 60   and name HB2 ))
     3.200      2.600      2.300 peak 18022 weight  0.10000E+01 volume  0.69853E+02 ppm1      3.227 ppm2      4.664
OR (18022)
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   (( segid "BrD " and resid 75   and name HG2 ))
   (( segid "BrD " and resid 72   and name HA  ))
OR (18022)
   (( segid "BrD " and resid 59   and name HG1 ))
   (( segid "BrD " and resid 60   and name HB2 ))
OR (18022)
   (( segid "BrD " and resid 59   and name HG3 ))
   (( segid "BrD " and resid 58   and name HB  ))
OR (18022)
   (( segid "BrD " and resid 59   and name HG1 ))
   (( segid "BrD " and resid 58   and name HB  ))
ASSI (18032)
   (( segid "BrD " and resid 75   and name HG2 ))
   (( segid "BrD " and resid 74   and name HB1 ))
      3.400      2.900      2.100 peak 18032 weight  0.10000E+01 volume  0.48637E+02 ppm1      3.226 ppm2      3.597
OR (18032)
   (( segid "BrD " and resid 59   and name HG1 ))
   (( segid "BrD " and resid 74   and name HB1 ))
OR (18032)
   (( segid "BrD " and resid 59   and name HG2 ))
   (( segid "BrD " and resid 74   and name HB1 ))
OR (18032)
   (( segid "BrD " and resid 59   and name HG1 ))
   (( segid "BrD " and resid 67   and name HB1 ))
ASSI (18252)
   (  segid "BrD " and resid 35   and name HE% )
   (( segid "BrD " and resid 60   and name HB2 ))
      3.500      3.100      2.000 peak 18252 weight  0.10000E+01 volume  0.44998E+02 ppm1      2.782 ppm2      4.631
OR (18252)
   (  segid "BrD " and resid 35   and name HE% )
   (( segid "BrD " and resid 56   and name HA  ))
ASSI (18332)
   (  segid "BrD " and resid 35   and name HE% )
   (( segid "BrD " and resid 25   and name HB  ))
      3.700      3.400      1.800 peak 18332 weight  0.10000E+01 volume  0.33097E+02 ppm1      2.782 ppm2      3.003
OR (18332)
   (  segid "BrD " and resid 35   and name HE% )
   (( segid "BrD " and resid 55   and name HB1 ))
ASSI (18342)
   (  segid "BrD " and resid 35   and name HE% )
   (( segid "BrD " and resid 35   and name HB1 ))
      1.700      1.700      2.800 peak 18342 weight  0.10000E+01 volume  0.31606E+04 ppm1      2.781 ppm2      2.841
OR (18342)
   (  segid "BrD " and resid 35   and name HE% )
   (( segid "BrD " and resid 57   and name HB2 ))
ASSI (18392)
   (  segid "BrD " and resid 35   and name HE% )
   (( segid "BrD " and resid 57   and name HD1 ))
      2.500      1.600      1.600 peak 18392 weight  0.10000E+01 volume  0.33173E+03 ppm1      2.782 ppm2      2.361
OR (18392)
   (  segid "BrD " and resid 35   and name HE% )
   (( segid "BrD " and resid 56   and name HG  ))
ASSI (18402)
   (  segid "BrD " and resid 35   and name HE% )
   (  segid "BrD " and resid 31   and name HB% )
      2.300      1.300      1.300 peak 18402 weight  0.10000E+01 volume  0.54118E+03 ppm1      2.782 ppm2      2.312
OR (18402)
   (  segid "BrD " and resid 35   and name HE% )
   (( segid "BrD " and resid 57   and name HD2 ))
OR (18402)
   (  segid "BrD " and resid 35   and name HE% )
   (( segid "BrD " and resid 56   and name HG  ))
ASSI (18432)
   (  segid "BrD " and resid 35   and name HE% )
   (( segid "BrD " and resid 57   and name HG1 ))
      2.800      2.000      2.000 peak 18432 weight  0.10000E+01 volume  0.16595E+03 ppm1      2.780 ppm2      2.118
OR (18432)
   (  segid "BrD " and resid 35   and name HE% )
   (( segid "BrD " and resid 26   and name HD1 ))
ASSI (18522)
   (  segid "BrD " and resid 75   and name HE% )
   (( segid "BrD " and resid 71   and name HA  ))
      2.600      1.700      1.700 peak 18522 weight  0.10000E+01 volume  0.24378E+03 ppm1      2.635 ppm2      4.663
OR (18522)
   (  segid "BrD " and resid 75   and name HE% )
   (( segid "BrD " and resid 14   and name HA  ))
ASSI (18532)
   (  segid "BrD " and resid 75   and name HE% )
   (( segid "BrD " and resid 110  and name HA  ))
      4.200      4.200      1.300 peak 18532 weight  0.10000E+01 volume  0.13873E+02 ppm1      2.633 ppm2      4.383
OR (18532)
   (  segid "BrD " and resid 75   and name HE% )
   (( segid "BrD " and resid 74   and name HA  ))
ASSI (18592)
   (  segid "BrD " and resid 75   and name HE% )
   (  segid "BrD " and resid 74   and name HE% )
      3.600      3.200      1.900 peak 18592 weight  0.10000E+01 volume  0.36365E+02 ppm1      2.634 ppm2      7.552
OR (18592)
   (  segid "BrD " and resid 75   and name HE% )
   (  segid "BrD " and resid 106  and name HD% )
ASSI (18822)
   (  segid "BrD " and resid 75   and name HE% )
   (( segid "BrD " and resid 116  and name HG12))
      3.300      2.700      2.200 peak 18822 weight  0.10000E+01 volume  0.58075E+02 ppm1      2.635 ppm2      1.588
OR (18822)
   (  segid "BrD " and resid 75   and name HE% )
   (  segid "BrD " and resid 21   and name HG2% )
ASSI (18832)
   (  segid "BrD " and resid 75   and name HE% )
   (  segid "BrD " and resid 63   and name HD1% )
      3.400      2.900      2.100 peak 18832 weight  0.10000E+01 volume  0.54622E+02 ppm1      2.635 ppm2      1.657
OR (18832)
   (  segid "BrD " and resid 75   and name HE% )
   (( segid "BrD " and resid 110  and name HG12))
OR (18832)
   (  segid "BrD " and resid 75   and name HE% )
   (( segid "BrD " and resid 21   and name HG12))
ASSI (18912)
   (  segid "BrD " and resid 75   and name HE% )
   (( segid "BrD " and resid 14   and name HB2 ))
      2.700      1.800      1.800 peak 18912 weight  0.10000E+01 volume  0.20227E+03 ppm1      2.635 ppm2      2.126
OR (18912)
   (  segid "BrD " and resid 75   and name HE% )
   (( segid "BrD " and resid 118  and name HG  ))
ASSI (18942)
   (  segid "BrD " and resid 75   and name HE% )
   (( segid "BrD " and resid 21   and name HG11))
      3.700      3.400      1.800 peak 18942 weight  0.10000E+01 volume  0.30880E+02 ppm1      2.636 ppm2      2.344
OR (18942)
   (  segid "BrD " and resid 75   and name HE% )
   (( segid "BrD " and resid 110  and name HB  ))
OR (18942)
   (  segid "BrD " and resid 75   and name HE% )
   (( segid "BrD " and resid 109  and name HB1 ))
ASSI (18962)
   (( segid "BrD " and resid 57   and name HB1 ))
   (( segid "BrD " and resid 37   and name HD1 ))
      3.100      2.400      2.400 peak 18962 weight  0.10000E+01 volume  0.84483E+02 ppm1      2.931 ppm2      4.289
OR (18962)
   (( segid "BrD " and resid 37   and name HB1 ))
   (( segid "BrD " and resid 37   and name HD1 ))
ASSI (19022)
   (( segid "BrD " and resid 75   and name HA  ))
   (( segid "BrD " and resid 78   and name HB2 ))
      2.500      1.600      1.600 peak 19022 weight  0.10000E+01 volume  0.30551E+03 ppm1      4.508 ppm2      1.043
OR (19022)
   (( segid "BrD " and resid 75   and name HA  ))
   (  segid "BrD " and resid 18   and name HD1% )
ASSI (19222)
   (  segid "BrD " and resid 43   and name HB% )
   (( segid "BrD " and resid 42   and name HB1 ))
      4.500      4.500      1.000 peak 19222 weight  0.10000E+01 volume  0.92899E+01 ppm1      1.697 ppm2      2.768
OR (19222)
   (  segid "BrD " and resid 43   and name HB% )
   (( segid "BrD " and resid 44   and name HG1 ))
ASSI (19332)
   (  segid "BrD " and resid 31   and name HB% )
   (( segid "BrD " and resid 26   and name HB1 ))
      3.600      3.200      1.900 peak 19332 weight  0.10000E+01 volume  0.33671E+02 ppm1      2.289 ppm2      2.466
OR (19332)
   (  segid "BrD " and resid 31   and name HB% )
   (( segid "BrD " and resid 21   and name HB  ))
ASSI (19342)
   (  segid "BrD " and resid 31   and name HB% )
   (( segid "BrD " and resid 56   and name HB1 ))
      3.300      2.700      2.200 peak 19342 weight  0.10000E+01 volume  0.60076E+02 ppm1      2.289 ppm2      2.719
OR (19342)
   (  segid "BrD " and resid 31   and name HB% )
   (( segid "BrD " and resid 29   and name HB1 ))
ASSI (19402)
   (  segid "BrD " and resid 31   and name HB% )
   (( segid "BrD " and resid 29   and name HA  ))
      3.600      3.200      1.900 peak 19402 weight  0.10000E+01 volume  0.34186E+02 ppm1      2.289 ppm2      4.810
OR (19402)
   (  segid "BrD " and resid 31   and name HB% )
   (( segid "BrD " and resid 24   and name HA  ))
ASSI (19452)
   (( segid "BrD " and resid 73   and name HB2 ))
   (( segid "BrD " and resid 72   and name HA  ))
      3.800      3.600      1.700 peak 19452 weight  0.10000E+01 volume  0.27108E+02 ppm1      2.486 ppm2      4.672
OR (19452)
   (( segid "BrD " and resid 73   and name HB2 ))
   (( segid "BrD " and resid 69   and name HA  ))
ASSI (19462)
   (( segid "BrD " and resid 73   and name HB1 ))
   (( segid "BrD " and resid 72   and name HA  ))
      3.900      3.800      1.600 peak 19462 weight  0.10000E+01 volume  0.22158E+02 ppm1      2.583 ppm2      4.672
OR (19462)
   (( segid "BrD " and resid 73   and name HB1 ))
   (( segid "BrD " and resid 69   and name HA  ))
ASSI (19472)
   (  segid "BrD " and resid 99   and name HB% )
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   (( segid "BrD " and resid 66   and name HB1 ))
      2.400      1.400      1.400 peak 19472 weight  0.10000E+01 volume  0.42620E+03 ppm1      2.190 ppm2      2.359
OR (19472)
   (  segid "BrD " and resid 99   and name HB% )
   (( segid "BrD " and resid 103  and name HB1 ))
ASSI (19562)
   (  segid "BrD " and resid 76   and name HB% )
   (( segid "BrD " and resid 51   and name HB1 ))
      1.800      1.800      2.700 peak 19562 weight  0.10000E+01 volume  0.21948E+04 ppm1      2.092 ppm2      1.946
OR (19562)
   (  segid "BrD " and resid 76   and name HB% )
   (( segid "BrD " and resid 116  and name HG11))
OR (19562)
   (  segid "BrD " and resid 76   and name HB% )
   (( segid "BrD " and resid 51   and name HG1 ))
ASSI (19712)
   (  segid "BrD " and resid 99   and name HB% )
   (( segid "BrD " and resid 98   and name HB1 ))
      3.300      2.700      2.200 peak 19712 weight  0.10000E+01 volume  0.62693E+02 ppm1      2.190 ppm2      3.988
OR (19712)
   (  segid "BrD " and resid 99   and name HB% )
   (( segid "BrD " and resid 96   and name HB1 ))
ASSI (19862)
   (( segid "BrD " and resid 102  and name HA  ))
   (( segid "BrD " and resid 105  and name HA  ))
      4.200      4.200      1.300 peak 19862 weight  0.10000E+01 volume  0.13941E+02 ppm1      4.261 ppm2      4.924
OR (19862)
   (( segid "BrD " and resid 102  and name HA  ))
   (( segid "BrD " and resid 30   and name HB1 ))
ASSI (19872)
   (( segid "BrD " and resid 102  and name HA  ))
   (  segid "BrD " and resid 105  and name HD% )
      2.700      1.800      1.800 peak 19872 weight  0.10000E+01 volume  0.22737E+03 ppm1      4.261 ppm2      7.779
OR (19872)
   (( segid "BrD " and resid 102  and name HA  ))
   (  segid "BrD " and resid 34   and name HE% )
ASSI (19892)
   (( segid "BrD " and resid 113  and name HA  ))
   (( segid "BrD " and resid 115  and name HG  ))
      3.600      3.200      1.900 peak 19892 weight  0.10000E+01 volume  0.36454E+02 ppm1      4.903 ppm2      2.133
OR (19892)
   (( segid "BrD " and resid 113  and name HA  ))
   (( segid "BrD " and resid 14   and name HB2 ))
ASSI (19932)
   (( segid "BrD " and resid 113  and name HA  ))
   (( segid "BrD " and resid 112  and name HA  ))
      3.400      2.900      2.100 peak 19932 weight  0.10000E+01 volume  0.55030E+02 ppm1      4.903 ppm2      4.598
OR (19932)
   (( segid "BrD " and resid 113  and name HA  ))
   (( segid "BrD " and resid 114  and name HA1 ))
ASSI (19972)
   (  segid "BrD " and resid 113  and name HB% )
   (  segid "BrD " and resid 75   and name HE% )
      3.400      2.900      2.100 peak 19972 weight  0.10000E+01 volume  0.53194E+02 ppm1      1.991 ppm2      2.662
OR (19972)
   (  segid "BrD " and resid 113  and name HB% )
   (( segid "BrD " and resid 112  and name HB1 ))
ASSI (20002)
   (  segid "BrD " and resid 113  and name HB% )
   (( segid "BrD " and resid 18   and name HG  ))
      2.700      1.800      1.800 peak 20002 weight  0.10000E+01 volume  0.18667E+03 ppm1      1.991 ppm2      2.304
OR (20002)
   (  segid "BrD " and resid 113  and name HB% )
   (( segid "BrD " and resid 110  and name HB  ))
OR (20002)
   (  segid "BrD " and resid 113  and name HB% )
   (( segid "BrD " and resid 109  and name HB1 ))
ASSI (20012)
   (  segid "BrD " and resid 113  and name HB% )
   (( segid "BrD " and resid 110  and name HB  ))
      3.900      3.800      1.600 peak 20012 weight  0.10000E+01 volume  0.22660E+02 ppm1      1.990 ppm2      2.369
OR (20012)
   (  segid "BrD " and resid 113  and name HB% )
   (( segid "BrD " and resid 109  and name HB1 ))
ASSI (20022)
   (  segid "BrD " and resid 113  and name HB% )
   (( segid "BrD " and resid 115  and name HG  ))
      3.300      2.700      2.200 peak 20022 weight  0.10000E+01 volume  0.61319E+02 ppm1      1.990 ppm2      2.135
OR (20022)
   (  segid "BrD " and resid 113  and name HB% )
   (( segid "BrD " and resid 14   and name HB2 ))
ASSI (20062)
   (( segid "BrD " and resid 110  and name HA  ))
   (  segid "BrD " and resid 116  and name HD1% )
      3.100      2.400      2.400 peak 20062 weight  0.10000E+01 volume  0.82911E+02 ppm1      4.411 ppm2      1.410
OR (20062)
   (( segid "BrD " and resid 110  and name HA  ))
   (( segid "BrD " and resid 109  and name HG1 ))
ASSI (20122)
   (  segid "BrD " and resid 113  and name HB% )
   (( segid "BrD " and resid 114  and name HA1 ))
      3.700      3.400      1.800 peak 20122 weight  0.10000E+01 volume  0.29578E+02 ppm1      1.994 ppm2      4.564
OR (20122)
   (  segid "BrD " and resid 113  and name HB% )
   (( segid "BrD " and resid 17   and name HA  ))
ASSI (20152)
   (  segid "BrD " and resid 113  and name HB% )
   (  segid "BrD " and resid 14   and name HD1% )
      2.700      1.800      1.800 peak 20152 weight  0.10000E+01 volume  0.21357E+03 ppm1      1.995 ppm2      1.425
OR (20152)
   (  segid "BrD " and resid 113  and name HB% )
   (  segid "BrD " and resid 14   and name HD2% )
OR (20152)
   (  segid "BrD " and resid 113  and name HB% )
   (( segid "BrD " and resid 109  and name HG1 ))
ASSI (20182)
   (( segid "BrD " and resid 17   and name HB  ))
   (( segid "BrD " and resid 14   and name HB2 ))
      3.400      2.900      2.100 peak 20182 weight  0.10000E+01 volume  0.54504E+02 ppm1      4.853 ppm2      2.149
OR (20182)
   (( segid "BrD " and resid 17   and name HB  ))
   (( segid "BrD " and resid 18   and name HB1 ))
OR (20182)
   (( segid "BrD " and resid 17   and name HB  ))
   (( segid "BrD " and resid 109  and name HB2 ))
ASSI (20202)
   (( segid "BrD " and resid 17   and name HB  ))
   (  segid "BrD " and resid 21   and name HD1% )
      4.300      4.300      1.200 peak 20202 weight  0.10000E+01 volume  0.12632E+02 ppm1      4.853 ppm2      1.222
OR (20202)
   (( segid "BrD " and resid 17   and name HB  ))
   (  segid "BrD " and resid 110  and name HG2% )
ASSI (20222)
   (  segid "BrD " and resid 17   and name HG2% )
   (( segid "BrD " and resid 14   and name HA  ))
      2.200      1.200      1.200 peak 20222 weight  0.10000E+01 volume  0.69704E+03 ppm1      1.747 ppm2      4.666
OR (20222)
   (  segid "BrD " and resid 17   and name HG2% )
   (( segid "BrD " and resid 109  and name HA  ))
OR (20222)
   (  segid "BrD " and resid 17   and name HG2% )
   (( segid "BrD " and resid 20   and name HB1 ))
ASSI (20262)
   (  segid "BrD " and resid 17   and name HG2% )
   (( segid "BrD " and resid 109  and name HB1 ))
      2.500      1.600      1.600 peak 20262 weight  0.10000E+01 volume  0.34655E+03 ppm1      1.747 ppm2      2.352
OR (20262)
   (  segid "BrD " and resid 17   and name HG2% )
   (( segid "BrD " and resid 21   and name HG11))
ASSI (20322)
   (( segid "BrD " and resid 20   and name HB1 ))
   (( segid "BrD " and resid 21   and name HG11))
      2.300      2.300      2.200 peak 20322 weight  0.10000E+01 volume  0.47335E+03 ppm1      4.656 ppm2      2.320
OR (20322)
   (( segid "BrD " and resid 20   and name HB1 ))
   (( segid "BrD " and resid 19   and name HB1 ))
OR (20322)
   (( segid "BrD " and resid 20   and name HB1 ))
   (( segid "BrD " and resid 109  and name HB1 ))
ASSI (20632)
   (( segid "BrD " and resid 112  and name HG2 ))
   (( segid "BrD " and resid 109  and name HD1 ))
      3.100      2.400      3.400 peak 20632 weight  0.10000E+01 volume  0.87177E+02 ppm1      2.832 ppm2      1.997
OR (20632)
   (( segid "BrD " and resid 112  and name HG2 ))
   (( segid "BrD " and resid 111  and name HG1 ))
OR (20632)
   (( segid "BrD " and resid 112  and name HG2 ))
   (  segid "BrD " and resid 113  and name HB% )
ASSI (20652)
   (( segid "BrD " and resid 111  and name HA  ))
   (  segid "BrD " and resid 115  and name HD1% )
      3.800      3.600      1.700 peak 20652 weight  0.10000E+01 volume  0.25940E+02 ppm1      4.656 ppm2      1.319
OR (20652)
   (( segid "BrD " and resid 104  and name HA  ))
   (  segid "BrD " and resid 102  and name HD2% )
OR (20652)
   (( segid "BrD " and resid 72   and name HA  ))
   (  segid "BrD " and resid 115  and name HD1% )
OR (20652)
   (( segid "BrD " and resid 104  and name HA  ))
   (  segid "BrD " and resid 102  and name HD1% )
OR (20652)
   (( segid "BrD " and resid 72   and name HA  ))
   (( segid "BrD " and resid 78   and name HB1 ))
ASSI (20662)
   (( segid "BrD " and resid 61   and name HA  ))
   (( segid "BrD " and resid 62   and name HB2 ))
      3.300      2.700      2.200 peak 20662 weight  0.10000E+01 volume  0.56653E+02 ppm1      4.656 ppm2      1.710
OR (20662)
   (( segid "BrD " and resid 67   and name HA  ))
   (( segid "BrD " and resid 62   and name HB2 ))
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OR (20662)
   (( segid "BrD " and resid 111  and name HA  ))
   (( segid "BrD " and resid 110  and name HG11))
ASSI (20672)
   (( segid "BrD " and resid 23   and name HA  ))
   (( segid "BrD " and resid 26   and name HG1 ))
      3.300      2.700      2.200 peak 20672 weight  0.10000E+01 volume  0.58313E+02 ppm1      4.656 ppm2      1.661
OR (20672)
   (( segid "BrD " and resid 23   and name HA  ))
   (  segid "BrD " and resid 22   and name HD1%)
OR (20672)
   (( segid "BrD " and resid 61   and name HA  ))
   (  segid "BrD " and resid 22   and name HD1%)
OR (20672)
   (( segid "BrD " and resid 61   and name HA  ))
   (( segid "BrD " and resid 62   and name HB2 ))
OR (20672)
   (( segid "BrD " and resid 23   and name HA  ))
   (  segid "BrD " and resid 25   and name HG2%)
OR (20672)
   (( segid "BrD " and resid 61   and name HA  ))
   (  segid "BrD " and resid 58   and name HG2%)
OR (20672)
   (( segid "BrD " and resid 67   and name HA  ))
   (( segid "BrD " and resid 62   and name HB2 ))
ASSI (20682)
   (( segid "BrD " and resid 67   and name HA  ))
   (  segid "BrD " and resid 69   and name HG1%)
      2.700      1.800      1.800 peak 20682 weight  0.10000E+01 volume  0.18983E+03 ppm1      4.656 ppm2      1.547
OR (20682)
   (( segid "BrD " and resid 67   and name HA  ))
   (  segid "BrD " and resid 73   and name HD1%)
ASSI (20792)
   (  segid "BrD " and resid 25   and name HG2%)
   (  segid "BrD " and resid 74   and name HE% )
      3.100      2.400      2.400 peak 20792 weight  0.10000E+01 volume  0.98567E+02 ppm1      1.648 ppm2      7.517
OR (20792)
   (  segid "BrD " and resid 25   and name HG2%)
   (  segid "BrD " and resid 106  and name HD% )
OR (20792)
   (  segid "BrD " and resid 58   and name HG2%)
   (  segid "BrD " and resid 74   and name HE% )
ASSI (20822)
   (  segid "BrD " and resid 25   and name HG2%)
   (  segid "BrD " and resid 34   and name HE% )
      3.300      2.700      2.200 peak 20822 weight  0.10000E+01 volume  0.60371E+02 ppm1      1.650 ppm2      7.791
OR (20822)
   (  segid "BrD " and resid 58   and name HG2%)
   (  segid "BrD " and resid 68   and name HD% )
ASSI (20842)
   (  segid "BrD " and resid 25   and name HG2%)
   (( segid "BrD " and resid 102  and name HA  ))
      3.600      3.200      1.900 peak 20842 weight  0.10000E+01 volume  0.35063E+02 ppm1      1.649 ppm2      4.282
OR (20842)
   (  segid "BrD " and resid 58   and name HG2%)
   (( segid "BrD " and resid 37   and name HD1 ))
ASSI (21092)
   (  segid "BrD " and resid 58   and name HG2%)
   (( segid "BrD " and resid 61   and name HG2 ))
      2.600      1.700      1.700 peak 21092 weight  0.10000E+01 volume  0.23144E+03 ppm1      1.648 ppm2      2.833
OR (21092)
   (  segid "BrD " and resid 58   and name HG2%)
   (( segid "BrD " and resid 61   and name HB1 ))
OR (21092)
   (  segid "BrD " and resid 58   and name HG2%)
   (( segid "BrD " and resid 57   and name HB2 ))
ASSI (21102)
   (  segid "BrD " and resid 25   and name HG2%)
   (( segid "BrD " and resid 56   and name HB1 ))
      2.500      1.600      1.600 peak 21102 weight  0.10000E+01 volume  0.34384E+03 ppm1      1.649 ppm2      2.700
OR (21102)
   (  segid "BrD " and resid 58   and name HG2%)
   (( segid "BrD " and resid 61   and name HB2 ))
OR (21102)
   (  segid "BrD " and resid 58   and name HG2%)
   (( segid "BrD " and resid 37   and name HG1 ))
OR (21102)
   (  segid "BrD " and resid 25   and name HG2%)
   (( segid "BrD " and resid 22   and name HB1 ))
ASSI (21112)
   (  segid "BrD " and resid 58   and name HG2%)
   (  segid "BrD " and resid 54   and name HE% )
      2.500      1.600      1.600 peak 21112 weight  0.10000E+01 volume  0.32059E+03 ppm1      1.649 ppm2      2.508
OR (21112)
   (  segid "BrD " and resid 25   and name HG2%)
   (( segid "BrD " and resid 26   and name HB1 ))
ASSI (21132)
   (( segid "BrD " and resid 83   and name HB  ))
   (( segid "BrD " and resid 79   and name HG1 ))
      5.000      5.000      0.500 peak 21132 weight  0.10000E+01 volume  0.54051E+01 ppm1      4.804 ppm2      3.028
OR (21132)
   (( segid "BrD " and resid 83   and name HB  ))
   (( segid "BrD " and resid 87   and name HG1 ))
ASSI (21152)
   (( segid "BrD " and resid 58   and name HA  ))
   (  segid "BrD " and resid 54   and name HE% )
      3.500      3.100      2.000 peak 21152 weight  0.10000E+01 volume  0.43944E+02 ppm1      4.459 ppm2      2.572
OR (21152)
   (( segid "BrD " and resid 83   and name HA  ))
   (( segid "BrD " and resid 87   and name HB2 ))
ASSI (21222)
   (  segid "BrD " and resid 83   and name HG2%)
   (( segid "BrD " and resid 80   and name HG1 ))
      3.000      2.200      2.200 peak 21222 weight  0.10000E+01 volume  0.98918E+02 ppm1      1.894 ppm2      2.366
OR (21222)
   (  segid "BrD " and resid 83   and name HG2%)
   (( segid "BrD " and resid 86   and name HB1 ))
ASSI (21382)
   (( segid "BrD " and resid 25   and name HB  ))
   (  segid "BrD " and resid 102  and name HD1%)
      5.400      5.400      0.100 peak 21382 weight  0.10000E+01 volume  0.33579E+01 ppm1      2.980 ppm2      1.273
OR (21382)
   (( segid "BrD " and resid 25   and name HB  ))
   (  segid "BrD " and resid 56   and name HD2%)
ASSI (21432)
   (  segid "BrD " and resid 25   and name HG1%)
   (  segid "BrD " and resid 31   and name HB% )
      3.300      2.700      2.200 peak 21432 weight  0.10000E+01 volume  0.60830E+02 ppm1      1.795 ppm2      2.330
OR (21432)
   (  segid "BrD " and resid 25   and name HG1%)
   (( segid "BrD " and resid 21   and name HG11))
ASSI (21442)
   (  segid "BrD " and resid 25   and name HG1%)
   (( segid "BrD " and resid 105  and name HB1 ))
      2.600      1.700      1.700 peak 21442 weight  0.10000E+01 volume  0.23532E+03 ppm1      1.796 ppm2      3.695
OR (21442)
   (  segid "BrD " and resid 25   and name HG1%)
   (( segid "BrD " and resid 105  and name HB2 ))
OR (21442)
   (  segid "BrD " and resid 25   and name HG1%)
   (( segid "BrD " and resid 106  and name HB2 ))
ASSI (21502)
   (( segid "BrD " and resid 38   and name HA  ))
   (( segid "BrD " and resid 39   and name HD1 ))
      3.600      3.200      1.900 peak 21502 weight  0.10000E+01 volume  0.37412E+02 ppm1      4.163 ppm2      2.291
OR (21502)
   (( segid "BrD " and resid 38   and name HA  ))
   (( segid "BrD " and resid 37   and name HB2 ))
ASSI (21552)
   (  segid "BrD " and resid 81   and name HG2%)
   (( segid "BrD " and resid 31   and name HA  ))
      3.000      2.200      2.200 peak 21552 weight  0.10000E+01 volume  0.11144E+03 ppm1      0.760 ppm2      4.981
OR (21552)
   (  segid "BrD " and resid 81   and name HG2%)
   (( segid "BrD " and resid 85   and name HA  ))
OR (21552)
   (  segid "BrD " and resid 81   and name HG2%)
   (( segid "BrD " and resid 77   and name HA  ))
ASSI (21572)
   (  segid "BrD " and resid 81   and name HG1%)
   (( segid "BrD " and resid 77   and name HA  ))
      3.200      2.600      2.300 peak 21572 weight  0.10000E+01 volume  0.78059E+02 ppm1      1.056 ppm2      4.972
OR (21572)
   (  segid "BrD " and resid 38   and name HG1%)
   (( segid "BrD " and resid 39   and name HA  ))
ASSI (21592)
   (  segid "BrD " and resid 38   and name HG1%)
   (( segid "BrD " and resid 53   and name HA  ))
      3.100      2.400      2.400 peak 21592 weight  0.10000E+01 volume  0.93082E+02 ppm1      1.056 ppm2      4.664
OR (21592)
   (  segid "BrD " and resid 81   and name HG1%)
   (( segid "BrD " and resid 80   and name HA  ))
OR (21592)
   (  segid "BrD " and resid 81   and name HG1%)
   (( segid "BrD " and resid 53   and name HA  ))
ASSI (21612)
   (  segid "BrD " and resid 38   and name HG1%)
   (( segid "BrD " and resid 37   and name HB1 ))
      3.600      3.600      1.700 peak 21612 weight  0.10000E+01 volume  0.25206E+02 ppm1      1.056 ppm2      2.966
OR (21612)
   (  segid "BrD " and resid 81   and name HG1%)
   (( segid "BrD " and resid 55   and name HB1 ))
ASSI (21652)
   (  segid "BrD " and resid 38   and name HG1%)
   (  segid "BrD " and resid 47   and name HE% )
      3.100      2.400      2.400 peak 21652 weight  0.10000E+01 volume  0.89355E+02 ppm1      1.056 ppm2      7.259
OR (21652)
   (  segid "BrD " and resid 81   and name HG1%)
   (  segid "BrD " and resid 82   and name HD% )
ASSI (21792)
   (( segid "BrD " and resid 81   and name HB  ))
   (( segid "BrD " and resid 82   and name HB2 ))
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    3.900      3.800      1.600 peak 21792 weight  0.10000E+01 volume  0.21639E+02 ppm1      2.042 ppm2      3.573
OR (21792)
  (( segid "BrD " and resid 81   and name HB  ))
  (( segid "BrD " and resid 84   and name HB1 ))
ASSI (21982)
  (  segid "BrD " and resid 50   and name HD1%)
  (( segid "BrD " and resid 49   and name HA  ))
    3.000      2.200      2.200 peak 21982 weight  0.10000E+01 volume  0.11219E+03 ppm1      1.153 ppm2      4.692
OR (21982)
  (  segid "BrD " and resid 50   and name HD1%)
  (( segid "BrD " and resid 53   and name HA  ))
OR (21982)
  (  segid "BrD " and resid 50   and name HD1%)
  (( segid "BrD " and resid 47   and name HA  ))
ASSI (22072)
  (  segid "BrD " and resid 50   and name HD1%)
  (  segid "BrD " and resid 38   and name HG1%)
    3.800      3.600      1.700 peak 22072 weight  0.10000E+01 volume  0.25153E+02 ppm1      1.154 ppm2      1.078
OR (22072)
  (  segid "BrD " and resid 50   and name HD1%)
  (  segid "BrD " and resid 81   and name HG1%)
ASSI (22432)
  (  segid "BrD " and resid 69   and name HG2%)
  (( segid "BrD " and resid 19   and name HB2 ))
    5.500      5.500      0.000 peak 22432 weight  0.10000E+01 volume  0.51248E+00 ppm1      1.425 ppm2      1.993
OR (22432)
  (  segid "BrD " and resid 69   and name HG2%)
  (  segid "BrD " and resid 113  and name HB% )
ASSI (22502)
  (  segid "BrD " and resid 25   and name HG2%)
  (  segid "BrD " and resid 35   and name HE% )
    2.900      2.100      2.100 peak 22502 weight  0.10000E+01 volume  0.14480E+03 ppm1      1.633 ppm2      2.752
OR (22502)
  (  segid "BrD " and resid 49   and name HG1%)
  (( segid "BrD " and resid 48   and name HB1 ))
OR (22502)
  (  segid "BrD " and resid 58   and name HG2%)
  (( segid "BrD " and resid 37   and name HG1 ))
ASSI (22622)
  (( segid "BrD " and resid 42   and name HA  ))
  (( segid "BrD " and resid 44   and name HD2 ))
    4.000      4.000      1.500 peak 22622 weight  0.10000E+01 volume  0.20863E+02 ppm1      5.051 ppm2      4.133
OR (22622)
  (( segid "BrD " and resid 42   and name HA  ))
  (( segid "BrD " and resid 38   and name HA  ))
ASSI (22802)
  (( segid "BrD " and resid 104  and name HB1 ))
  (( segid "BrD " and resid 105  and name HB2 ))
    3.200      2.600      2.300 peak 22802 weight  0.10000E+01 volume  0.76681E+02 ppm1      2.536 ppm2      3.662
OR (22802)
  (( segid "BrD " and resid 104  and name HB1 ))
  (( segid "BrD " and resid 107  and name HB1 ))
ASSI (22862)
  (( segid "BrD " and resid 44   and name HE1 ))
  (( segid "BrD " and resid 19   and name HA  ))
    3.600      3.200      1.900 peak 22862 weight  0.10000E+01 volume  0.38596E+02 ppm1      3.573 ppm2      4.285
OR (22862)
  (( segid "BrD " and resid 57   and name HE1 ))
  (( segid "BrD " and resid 37   and name HD1 ))
ASSI (22912)
  (( segid "BrD " and resid 60   and name HB1 ))
  (( segid "BrD " and resid 22   and name HB2 ))
    4.100      4.100      1.400 peak 22912 weight  0.10000E+01 volume  0.16339E+02 ppm1      5.001 ppm2      2.312
OR (22912)
  (( segid "BrD " and resid 60   and name HB1 ))
  (( segid "BrD " and resid 56   and name HG  ))
ASSI (23002)
  (( segid "BrD " and resid 37   and name HD1 ))
  (( segid "BrD " and resid 57   and name HB1 ))
    3.100      2.400      2.400 peak 23002 weight  0.10000E+01 volume  0.82823E+02 ppm1      4.285 ppm2      2.966
OR (23002)
  (( segid "BrD " and resid 37   and name HD1 ))
  (( segid "BrD " and resid 37   and name HB1 ))
OR (23002)
  (( segid "BrD " and resid 44   and name HD1 ))
  (( segid "BrD " and resid 44   and name HB1 ))
ASSI (23042)
  (( segid "BrD " and resid 37   and name HD1 ))
  (( segid "BrD " and resid 37   and name HG2 ))
    2.000      1.000      1.000 peak 23042 weight  0.10000E+01 volume  0.14416E+04 ppm1      4.261 ppm2      2.621
OR (23042)
  (( segid "BrD " and resid 8    and name HD2 ))
  (( segid "BrD " and resid 8    and name HG1 ))
ASSI (23052)
  (( segid "BrD " and resid 8    and name HD1 ))
  (( segid "BrD " and resid 8    and name HB2 ))
    3.600      3.200      1.900 peak 23052 weight  0.10000E+01 volume  0.37937E+02 ppm1      4.409 ppm2      2.499
OR (23052)
  (( segid "BrD " and resid 8    and name HD1 ))
  (( segid "BrD " and resid 7    and name HB2 ))
ASSI (23212)
  (( segid "BrD " and resid 44   and name HG2 ))
  (( segid "BrD " and resid 44   and name HA  ))
    3.100      2.400      2.400 peak 23212 weight  0.10000E+01 volume  0.93659E+02 ppm1      2.635 ppm2      5.120
OR (23212)
  (( segid "BrD " and resid 8    and name HG1 ))
  (( segid "BrD " and resid 7    and name HA  ))
ASSI (23252)
  (( segid "BrD " and resid 11   and name HG1 ))
  (  segid "BrD " and resid 69   and name HG2%)
    3.000      2.200      2.200 peak 23252 weight  0.10000E+01 volume  0.10852E+03 ppm1      2.635 ppm2      1.417
OR (23252)
  (( segid "BrD " and resid 11   and name HG1 ))
  (  segid "BrD " and resid 14   and name HD2%)
ASSI (23382)
  (( segid "BrD " and resid 100  and name HA  ))
  (( segid "BrD " and resid 101  and name HA  ))
    5.500      5.500      0.000 peak 23382 weight  0.10000E+01 volume  0.24494E+01 ppm1      4.952 ppm2      4.256
OR (23382)
  (( segid "BrD " and resid 6    and name HA  ))
  (( segid "BrD " and resid 8    and name HD2 ))
ASSI (23392)
  (( segid "BrD " and resid 100  and name HA  ))
  (( segid "BrD " and resid 99   and name HA  ))
    3.200      2.600      2.300 peak 23392 weight  0.10000E+01 volume  0.72079E+02 ppm1      4.952 ppm2      4.444
OR (23392)
  (( segid "BrD " and resid 6    and name HA  ))
  (( segid "BrD " and resid 8    and name HD1 ))
ASSI (23512)
  (( segid "BrD " and resid 10   and name HA  ))
  (( segid "BrD " and resid 11   and name HA  ))
    3.400      2.900      2.100 peak 23512 weight  0.10000E+01 volume  0.53886E+02 ppm1      5.477 ppm2      4.939
OR (23512)
  (( segid "BrD " and resid 10   and name HA  ))
  (( segid "BrD " and resid 9    and name HA  ))
ASSI (23582)
  (( segid "BrD " and resid 12   and name HA  ))
  (( segid "BrD " and resid 15   and name HA  ))
    3.600      3.200      1.900 peak 23582 weight  0.10000E+01 volume  0.33831E+02 ppm1      5.297 ppm2      4.627
OR (23582)
  (( segid "BrD " and resid 12   and name HA  ))
  (( segid "BrD " and resid 16   and name HB1 ))
OR (23582)
  (( segid "BrD " and resid 12   and name HA  ))
  (( segid "BrD " and resid 14   and name HA  ))
ASSI (23682)
  (( segid "BrD " and resid 14   and name HA  ))
  (  segid "BrD " and resid 18   and name HD1%)
    3.300      2.700      2.200 peak 23682 weight  0.10000E+01 volume  0.67221E+02 ppm1      4.656 ppm2      1.083
OR (23682)
  (( segid "BrD " and resid 80   and name HA  ))
  (  segid "BrD " and resid 81   and name HG1%)
ASSI (23772)
  (  segid "BrD " and resid 14   and name HD2%)
  (( segid "BrD " and resid 15   and name HA  ))
    2.400      1.400      1.400 peak 23772 weight  0.10000E+01 volume  0.36871E+03 ppm1      1.400 ppm2      4.574
OR (23772)
  (( segid "BrD " and resid 109  and name HG1 ))
  (( segid "BrD " and resid 17   and name HA  ))
ASSI (23792)
  (  segid "BrD " and resid 14   and name HD2%)
  (( segid "BrD " and resid 18   and name HA  ))
    3.900      3.800      1.600 peak 23792 weight  0.10000E+01 volume  0.23631E+02 ppm1      1.401 ppm2      3.889
OR (23792)
  (( segid "BrD " and resid 109  and name HG1 ))
  (( segid "BrD " and resid 18   and name HA  ))
ASSI (23872)
  (( segid "BrD " and resid 18   and name HA  ))
  (  segid "BrD " and resid 74   and name HE% )
    2.900      2.100      2.100 peak 23872 weight  0.10000E+01 volume  0.13092E+03 ppm1      3.866 ppm2      7.534
OR (23872)
  (( segid "BrD " and resid 18   and name HA  ))
  (  segid "BrD " and resid 106  and name HD% )
ASSI (23892)
  (( segid "BrD " and resid 18   and name HA  ))
  (( segid "BrD " and resid 15   and name HA  ))
    2.900      2.100      2.100 peak 23892 weight  0.10000E+01 volume  0.13327E+03 ppm1      3.867 ppm2      4.631
OR (23892)
  (( segid "BrD " and resid 18   and name HA  ))
  (( segid "BrD " and resid 20   and name HB1 ))
OR (23892)
  (( segid "BrD " and resid 18   and name HA  ))
  (( segid "BrD " and resid 14   and name HA  ))
ASSI (23902)
  (( segid "BrD " and resid 18   and name HA  ))
  (( segid "BrD " and resid 17   and name HA  ))
    3.800      3.600      1.700 peak 23902 weight  0.10000E+01 volume  0.26018E+02 ppm1      3.867 ppm2      4.541
OR (23902)
  (( segid "BrD " and resid 18   and name HA  ))
  (( segid "BrD " and resid 106  and name HA  ))
ASSI (23912)
  (( segid "BrD " and resid 18   and name HB1 ))
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   ( segid "BrD " and resid 14   and name HD2%)
     3.400      3.900      2.100 peak 23912 weight  0.10000E+01 volume  0.53948E+02 ppm1      2.140 ppm2      1.433
OR (23912)
   (( segid "BrD " and resid 18   and name HB1 ))
   ( segid "BrD " and resid 69   and name HG2%)
ASSI (23942)
   (( segid "BrD " and resid 18   and name HB2 ))
   ( segid "BrD " and resid 14   and name HD2%)
     4.100      4.100      1.400 peak 23942 weight  0.10000E+01 volume  0.16641E+02 ppm1      0.911 ppm2      1.415
OR (23942)
   (( segid "BrD " and resid 18   and name HB2 ))
   ( segid "BrD " and resid 69   and name HG2%)
ASSI (24102)
   ( segid "BrD " and resid 18   and name HD2%)
   ( segid "BrD " and resid 21   and name HG2%)
     5.500      5.500      0.000 peak 24102 weight  0.10000E+01 volume  0.18200E+00 ppm1      0.415 ppm2      1.596
OR (24102)
   ( segid "BrD " and resid 18   and name HD2%)
   ( segid "BrD " and resid 22   and name HD2%)
ASSI (24112)
   ( segid "BrD " and resid 18   and name HD2%)
   ( segid "BrD " and resid 115  and name HD1%)
     2.800      2.000      2.000 peak 24112 weight  0.10000E+01 volume  0.15952E+03 ppm1      0.416 ppm2      1.377
OR (24112)
   ( segid "BrD " and resid 18   and name HD2%)
   ( segid "BrD " and resid 14   and name HD2%)
OR (24112)
   ( segid "BrD " and resid 18   and name HD2%)
   ( segid "BrD " and resid 14   and name HD1%)
ASSI (24122)
   ( segid "BrD " and resid 18   and name HD2%)
   ( segid "BrD " and resid 113  and name HB% )
     3.900      3.800      1.600 peak 24122 weight  0.10000E+01 volume  0.21517E+02 ppm1      0.415 ppm2      1.986
OR (24122)
   ( segid "BrD " and resid 18   and name HD2%)
   (( segid "BrD " and resid 19   and name HB2 ))
ASSI (24292)
   ( segid "BrD " and resid 18   and name HD2%)
   (( segid "BrD " and resid 106  and name HB2 ))
     3.900      3.800      1.600 peak 24292 weight  0.10000E+01 volume  0.23222E+02 ppm1      0.416 ppm2      3.650
OR (24292)
   ( segid "BrD " and resid 18   and name HD2%)
   (( segid "BrD " and resid 68   and name HB1 ))
OR (24292)
   ( segid "BrD " and resid 18   and name HD2%)
   (( segid "BrD " and resid 15   and name HB2 ))
ASSI (24492)
   ( segid "BrD " and resid 63   and name HD1%)
   (( segid "BrD " and resid 68   and name HB1 ))
     2.800      2.000      2.000 peak 24492 weight  0.10000E+01 volume  0.15293E+03 ppm1      1.649 ppm2      3.671
OR (24492)
   ( segid "BrD " and resid 63   and name HD1%)
   (( segid "BrD " and resid 15   and name HB2 ))
ASSI (24502)
   ( segid "BrD " and resid 63   and name HD1%)
   (( segid "BrD " and resid 66   and name HD2 ))
     3.000      2.200      2.200 peak 24502 weight  0.10000E+01 volume  0.10614E+03 ppm1      1.649 ppm2      3.614
OR (24502)
   ( segid "BrD " and resid 63   and name HD1%)
   (( segid "BrD " and resid 64   and name HE1 ))
ASSI (24532)
   ( segid "BrD " and resid 63   and name HD1%)
   (( segid "BrD " and resid 16   and name HA  ))
     3.500      3.100      2.000 peak 24532 weight  0.10000E+01 volume  0.45951E+02 ppm1      1.649 ppm2      4.516
OR (24532)
   ( segid "BrD " and resid 63   and name HD1%)
   (( segid "BrD " and resid 17   and name HA  ))
ASSI (24602)
   ( segid "BrD " and resid 63   and name HD2%)
   (( segid "BrD " and resid 19   and name HE1 ))
     3.400      2.900      2.100 peak 24602 weight  0.10000E+01 volume  0.54742E+02 ppm1      1.500 ppm2      3.524
OR (24602)
   ( segid "BrD " and resid 63   and name HD2%)
   (( segid "BrD " and resid 68   and name HB2 ))
ASSI (24692)
   (( segid "BrD " and resid 19   and name HA  ))
   (( segid "BrD " and resid 22   and name HG  ))
     3.000      2.200      2.200 peak 24692 weight  0.10000E+01 volume  0.10572E+03 ppm1      4.310 ppm2      2.393
OR (24692)
   (( segid "BrD " and resid 19   and name HA  ))
   (( segid "BrD " and resid 64   and name HD1 ))
ASSI (24712)
   (( segid "BrD " and resid 19   and name HA  ))
   (( segid "BrD " and resid 23   and name HA  ))
     3.700      3.400      1.800 peak 24712 weight  0.10000E+01 volume  0.31255E+02 ppm1      4.310 ppm2      4.677
OR (24712)
   (( segid "BrD " and resid 19   and name HA  ))
   (( segid "BrD " and resid 22   and name HA  ))
OR (24712)
   (( segid "BrD " and resid 19   and name HA  ))
   (( segid "BrD " and resid 20   and name HB1 ))
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ASSI (24722)
   (( segid "BrD " and resid 19   and name HB2 ))
   (( segid "BrD " and resid 15   and name HA  ))
     3.800      3.600      1.700 peak 24722 weight  0.10000E+01 volume  0.24706E+02 ppm1      1.989 ppm2      4.974
OR (24722)
   (( segid "BrD " and resid 19   and name HB2 ))
   (( segid "BrD " and resid 16   and name HB1 ))
ASSI (24732)
   (( segid "BrD " and resid 19   and name HB2 ))
   (( segid "BrD " and resid 15   and name HA  ))
     3.800      3.600      1.700 peak 24732 weight  0.10000E+01 volume  0.28161E+02 ppm1      1.989 ppm2      4.631
OR (24732)
   (( segid "BrD " and resid 19   and name HB2 ))
   (( segid "BrD " and resid 20   and name HB1 ))
ASSI (24772)
   (( segid "BrD " and resid 19   and name HG1 ))
   (( segid "BrD " and resid 20   and name HA  ))
     4.200      4.200      1.300 peak 24772 weight  0.10000E+01 volume  0.15236E+02 ppm1      1.895 ppm2      4.891
OR (24772)
   (( segid "BrD " and resid 86   and name HG1 ))
   (( segid "BrD " and resid 87   and name HA  ))
OR (24772)
   (( segid "BrD " and resid 19   and name HG1 ))
   (( segid "BrD " and resid 64   and name HA  ))
ASSI (24822)
   (( segid "BrD " and resid 19   and name HD1 ))
   (( segid "BrD " and resid 15   and name HA  ))
     4.100      4.100      1.400 peak 24822 weight  0.10000E+01 volume  0.16533E+02 ppm1      2.190 ppm2      4.643
OR (24822)
   (( segid "BrD " and resid 19   and name HD1 ))
   (( segid "BrD " and resid 20   and name HB1 ))
ASSI (24852)
   (( segid "BrD " and resid 97   and name HE1 ))
   (( segid "BrD " and resid 97   and name HA  ))
     2.000      2.000      2.500 peak 24852 weight  0.10000E+01 volume  0.10950E+04 ppm1      3.571 ppm2      4.802
OR (24852)
   (( segid "BrD " and resid 57   and name HE1 ))
   (( segid "BrD " and resid 57   and name HA  ))
ASSI (24982)
   (( segid "BrD " and resid 21   and name HA  ))
   ( segid "BrD " and resid 106  and name HD% )
     3.600      3.200      1.900 peak 24982 weight  0.10000E+01 volume  0.38794E+02 ppm1      4.358 ppm2      7.617
OR (24982)
   (( segid "BrD " and resid 33   and name HA  ))
   ( segid "BrD " and resid 95   and name HD% )
ASSI (24992)
   (( segid "BrD " and resid 21   and name HA  ))
   (( segid "BrD " and resid 22   and name HA  ))
     2.000      2.000      2.500 peak 24992 weight  0.10000E+01 volume  0.12806E+04 ppm1      4.360 ppm2      4.671
OR (24992)
   (( segid "BrD " and resid 21   and name HA  ))
   (( segid "BrD " and resid 20   and name HB1 ))
ASSI (25052)
   (( segid "BrD " and resid 21   and name HG12))
   (( segid "BrD " and resid 18   and name HB1 ))
     3.500      3.100      2.000 peak 25052 weight  0.10000E+01 volume  0.40558E+02 ppm1      1.648 ppm2      2.141
OR (25052)
   (( segid "BrD " and resid 21   and name HG12))
   (( segid "BrD " and resid 109  and name HB2 ))
ASSI (25112)
   (( segid "BrD " and resid 21   and name HG12))
   (( segid "BrD " and resid 109  and name HG1 ))
     3.900      3.800      1.600 peak 25112 weight  0.10000E+01 volume  0.24225E+02 ppm1      1.648 ppm2      1.387
OR (25112)
   (( segid "BrD " and resid 21   and name HG12))
   ( segid "BrD " and resid 115  and name HD1%)
OR (25112)
   (( segid "BrD " and resid 21   and name HG12))
   ( segid "BrD " and resid 14   and name HD2%)
ASSI (25152)
   ( segid "BrD " and resid 21   and name HD1%)
   (( segid "BrD " and resid 106  and name HA  ))
     2.600      1.700      1.700 peak 25152 weight  0.10000E+01 volume  0.24691E+03 ppm1      1.205 ppm2      4.848
OR (25152)
   ( segid "BrD " and resid 21   and name HD1%)
   (( segid "BrD " and resid 17   and name HA  ))
OR (25152)
   ( segid "BrD " and resid 21   and name HD1%)
   (( segid "BrD " and resid 75   and name HA  ))
ASSI (25162)
   ( segid "BrD " and resid 21   and name HD1%)
   (( segid "BrD " and resid 20   and name HA  ))
     5.500      5.500      0.000 peak 25162 weight  0.10000E+01 volume  0.64481E-01 ppm1      1.205 ppm2      4.907
OR (25162)
   ( segid "BrD " and resid 21   and name HD1%)
   (( segid "BrD " and resid 105  and name HA  ))
OR (25162)
   ( segid "BrD " and resid 21   and name HD1%)
   (( segid "BrD " and resid 59   and name HA  ))
ASSI (25172)
   ( segid "BrD " and resid 21   and name HD1%)
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  (( segid "BrD " and resid 17   and name HB  ))
     3.100      2.400      2.400 peak 25172 weight  0.10000E+01 volume  0.95979E+02 ppm1      1.205 ppm2      4.863
OR (25172)
   (  segid "BrD " and resid 21   and name HD1%)
   (( segid "BrD " and resid 20   and name HA  ))
ASSI (25182)
   (  segid "BrD " and resid 21   and name HD1%)
   (  segid "BrD " and resid 74   and name HE% )
     2.600      1.700      1.700 peak 25182 weight  0.10000E+01 volume  0.25847E+03 ppm1      1.204 ppm2      7.536
OR (25182)
   (  segid "BrD " and resid 21   and name HD1%)
   (  segid "BrD " and resid 106  and name HD% )
ASSI (25392)
   (( segid "BrD " and resid 98   and name HA  ))
   (( segid "BrD " and resid 101  and name HA  ))
     3.400      2.900      2.100 peak 25392 weight  0.10000E+01 volume  0.50125E+02 ppm1      4.804 ppm2      4.265
OR (25392)
   (( segid "BrD " and resid 98   and name HA  ))
   (( segid "BrD " and resid 102  and name HA  ))
ASSI (25602)
   (  segid "BrD " and resid 21   and name HG2%)
   (( segid "BrD " and resid 20   and name HB1 ))
     3.400      2.900      2.100 peak 25602 weight  0.10000E+01 volume  0.54447E+02 ppm1      1.596 ppm2      4.657
OR (25602)
   (  segid "BrD " and resid 21   and name HG2%)
   (( segid "BrD " and resid 109  and name HA  ))
ASSI (25622)
   (  segid "BrD " and resid 21   and name HG2%)
   (( segid "BrD " and resid 105  and name HB1 ))
     3.400      2.900      2.100 peak 25622 weight  0.10000E+01 volume  0.55968E+02 ppm1      1.599 ppm2      3.736
OR (25622)
   (  segid "BrD " and resid 101  and name HG2%)
   (( segid "BrD " and resid 105  and name HB1 ))
ASSI (25632)
   (  segid "BrD " and resid 21   and name HG2%)
   (( segid "BrD " and resid 106  and name HB2 ))
     4.400      4.400      1.100 peak 25632 weight  0.10000E+01 volume  0.10843E+02 ppm1      1.599 ppm2      3.662
OR (25632)
   (  segid "BrD " and resid 21   and name HG2%)
   (( segid "BrD " and resid 105  and name HB2 ))
ASSI (25672)
   (  segid "BrD " and resid 101  and name HD1%)
   (( segid "BrD " and resid 97   and name HB1 ))
     3.100      2.400      2.400 peak 25672 weight  0.10000E+01 volume  0.84040E+02 ppm1      1.550 ppm2      2.702
OR (25672)
   (  segid "BrD " and resid 101  and name HD1%)
   (( segid "BrD " and resid 29   and name HB1 ))
ASSI (25692)
   (  segid "BrD " and resid 101  and name HD1%)
   (( segid "BrD " and resid 97   and name HG2 ))
     3.800      3.600      1.700 peak 25692 weight  0.10000E+01 volume  0.27614E+02 ppm1      1.550 ppm2      2.167
OR (25692)
   (  segid "BrD " and resid 101  and name HD1%)
   (  segid "BrD " and resid 99   and name HB% )
OR (25692)
   (  segid "BrD " and resid 101  and name HD1%)
   (( segid "BrD " and resid 33   and name HD2 ))
ASSI (25702)
   (  segid "BrD " and resid 21   and name HG2%)
   (  segid "BrD " and resid 75   and name HE% )
     4.300      4.300      1.200 peak 25702 weight  0.10000E+01 volume  0.11881E+02 ppm1      1.599 ppm2      2.654
OR (25702)
   (  segid "BrD " and resid 21   and name HG2%)
   (( segid "BrD " and resid 22   and name HB1 ))
OR (25702)
   (  segid "BrD " and resid 101  and name HG2%)
   (( segid "BrD " and resid 97   and name HB1 ))
ASSI (25732)
   (  segid "BrD " and resid 101  and name HG2%)
   (( segid "BrD " and resid 102  and name HB1 ))
     2.600      1.700      1.700 peak 25732 weight  0.10000E+01 volume  0.25581E+03 ppm1      1.599 ppm2      2.011
OR (25732)
   (  segid "BrD " and resid 21   and name HG2%)
   (( segid "BrD " and resid 109  and name HD1 ))
ASSI (25772)
   (  segid "BrD " and resid 21   and name HG2%)
   (  segid "BrD " and resid 18   and name HD1%)
     3.200      2.600      2.300 peak 25772 weight  0.10000E+01 volume  0.75349E+02 ppm1      1.599 ppm2      1.059
OR (25772)
   (  segid "BrD " and resid 21   and name HG2%)
   (( segid "BrD " and resid 78   and name HB2 ))
OR (25772)
   (  segid "BrD " and resid 21   and name HG2%)
   (  segid "BrD " and resid 81   and name HG1%)
ASSI (25832)
   (( segid "BrD " and resid 110  and name HB  ))
   (( segid "BrD " and resid 108  and name HA  ))
     3.800      3.600      1.700 peak 25832 weight  0.10000E+01 volume  0.26102E+02 ppm1      2.338 ppm2      4.823
OR (25832)
   (( segid "BrD " and resid 110  and name HB  ))
   (( segid "BrD " and resid 115  and name HA  ))
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ASSI (25862)
   (  segid "BrD " and resid 110  and name HG2%)
   (( segid "BrD " and resid 114  and name HA2 ))
     3.100      2.400      2.400 peak 25862 weight  0.10000E+01 volume  0.90131E+02 ppm1      1.254 ppm2      4.509
OR (25862)
   (  segid "BrD " and resid 110  and name HG2%)
   (( segid "BrD " and resid 75   and name HA  ))
ASSI (25872)
   (  segid "BrD " and resid 110  and name HD1%)
   (( segid "BrD " and resid 14   and name HA  ))
     2.800      2.000      2.000 peak 25872 weight  0.10000E+01 volume  0.15256E+03 ppm1      1.154 ppm2      4.655
OR (25872)
   (  segid "BrD " and resid 110  and name HD1%)
   (( segid "BrD " and resid 71   and name HA  ))
OR (25872)
   (  segid "BrD " and resid 110  and name HD1%)
   (( segid "BrD " and resid 111  and name HA  ))
OR (25872)
   (  segid "BrD " and resid 110  and name HD1%)
   (( segid "BrD " and resid 109  and name HA  ))
ASSI (25882)
   (  segid "BrD " and resid 110  and name HG2%)
   (( segid "BrD " and resid 115  and name HA  ))
     2.800      2.000      2.000 peak 25882 weight  0.10000E+01 volume  0.15787E+03 ppm1      1.253 ppm2      4.824
OR (25882)
   (  segid "BrD " and resid 110  and name HG2%)
   (( segid "BrD " and resid 116  and name HA  ))
ASSI (25892)
   (  segid "BrD " and resid 110  and name HD1%)
   (( segid "BrD " and resid 17   and name HB  ))
     3.100      2.400      2.400 peak 25892 weight  0.10000E+01 volume  0.95882E+02 ppm1      1.154 ppm2      4.824
OR (25892)
   (  segid "BrD " and resid 110  and name HD1%)
   (( segid "BrD " and resid 115  and name HA  ))
ASSI (25902)
   (  segid "BrD " and resid 110  and name HD1%)
   (( segid "BrD " and resid 106  and name HA  ))
     3.000      2.200      2.200 peak 25902 weight  0.10000E+01 volume  0.11502E+03 ppm1      1.154 ppm2      4.568
OR (25902)
   (  segid "BrD " and resid 110  and name HD1%)
   (( segid "BrD " and resid 17   and name HA  ))
OR (25902)
   (  segid "BrD " and resid 110  and name HD1%)
   (( segid "BrD " and resid 114  and name HA1 ))
ASSI (26022)
   (  segid "BrD " and resid 110  and name HD1%)
   (( segid "BrD " and resid 106  and name HB2 ))
     3.200      2.600      2.300 peak 26022 weight  0.10000E+01 volume  0.70430E+02 ppm1      1.154 ppm2      3.670
OR (26022)
   (  segid "BrD " and resid 110  and name HD1%)
   (( segid "BrD " and resid 107  and name HB1 ))
ASSI (26042)
   (  segid "BrD " and resid 110  and name HG2%)
   (( segid "BrD " and resid 107  and name HB1 ))
     3.600      3.200      1.900 peak 26042 weight  0.10000E+01 volume  0.38059E+02 ppm1      1.251 ppm2      3.671
OR (26042)
   (  segid "BrD " and resid 110  and name HG2%)
   (( segid "BrD " and resid 106  and name HB2 ))
ASSI (26202)
   (  segid "BrD " and resid 116  and name HG2%)
   (( segid "BrD " and resid 76   and name HA  ))
     2.600      1.700      1.700 peak 26202 weight  0.10000E+01 volume  0.28885E+03 ppm1      1.401 ppm2      4.655
OR (26202)
   (  segid "BrD " and resid 116  and name HG2%)
   (( segid "BrD " and resid 72   and name HA  ))
ASSI (26312)
   (  segid "BrD " and resid 116  and name HD1%)
   (( segid "BrD " and resid 76   and name HA  ))
     3.800      3.600      1.700 peak 26312 weight  0.10000E+01 volume  0.26059E+02 ppm1      1.401 ppm2      4.655
OR (26312)
   (  segid "BrD " and resid 116  and name HD1%)
   (( segid "BrD " and resid 118  and name HA  ))
OR (26312)
   (  segid "BrD " and resid 116  and name HD1%)
   (( segid "BrD " and resid 111  and name HA  ))
OR (26312)
   (  segid "BrD " and resid 116  and name HD1%)
   (( segid "BrD " and resid 71   and name HA  ))
OR (26312)
   (  segid "BrD " and resid 116  and name HD1%)
   (( segid "BrD " and resid 72   and name HA  ))
ASSI (26352)
   (  segid "BrD " and resid 116  and name HG2%)
   (( segid "BrD " and resid 79   and name HA  ))
     3.400      3.200      1.900 peak 26352 weight  0.10000E+01 volume  0.36722E+02 ppm1      1.400 ppm2      4.428
OR (26352)
   (  segid "BrD " and resid 116  and name HG2%)
   (( segid "BrD " and resid 107  and name HA  ))
ASSI (26362)
   (  segid "BrD " and resid 116  and name HD1%)
   (( segid "BrD " and resid 107  and name HB1 ))
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    3.800      3.600      1.700 peak 26362 weight  0.10000E+01 volume  0.28562E+02 ppm1      1.401 ppm2      3.662
OR (26362)
  (  segid "BrD " and resid 116  and name HD1%)
  (( segid "BrD " and resid 106  and name HB2 ))
ASSI (26512)
  (( segid "BrD " and resid 116  and name HB  ))
  (( segid "BrD " and resid 76   and name HA  ))
    3.300      2.700      2.200 peak 26512 weight  0.10000E+01 volume  0.66907E+02 ppm1      2.410 ppm2      4.655
OR (26512)
  (( segid "BrD " and resid 116  and name HB  ))
  (( segid "BrD " and resid 118  and name HA  ))
OR (26512)
  (( segid "BrD " and resid 116  and name HB  ))
  (( segid "BrD " and resid 72   and name HA  ))
ASSI (27012)
  (( segid "BrD " and resid 89   and name HA  ))
  (( segid "BrD " and resid 88   and name HA  ))
    3.600      3.200      1.900 peak 27012 weight  0.10000E+01 volume  0.33743E+02 ppm1      5.642 ppm2      5.005
OR (27012)
  (( segid "BrD " and resid 89   and name HA  ))
  (( segid "BrD " and resid 93   and name HB1 ))
ASSI (27292)
  (( segid "BrD " and resid 80   and name HG1 ))
  (( segid "BrD " and resid 52   and name HB1 ))
    3.300      2.700      2.200 peak 27292 weight  0.10000E+01 volume  0.61197E+02 ppm1      2.341 ppm2      3.649
OR (27292)
  (( segid "BrD " and resid 73   and name HG  ))
  (( segid "BrD " and resid 68   and name HB1 ))
ASSI (27302)
  (( segid "BrD " and resid 80   and name HG1 ))
  (( segid "BrD " and resid 77   and name HB1 ))
    4.600      4.600      0.900 peak 27302 weight  0.10000E+01 volume  0.87654E+01 ppm1      2.341 ppm2      3.311
OR (27302)
  (( segid "BrD " and resid 73   and name HG  ))
  (( segid "BrD " and resid 77   and name HB1 ))
OR (27302)
  (( segid "BrD " and resid 73   and name HG  ))
  (( segid "BrD " and resid 54   and name HG1 ))
OR (27302)
  (( segid "BrD " and resid 56   and name HG  ))
  (( segid "BrD " and resid 54   and name HG1 ))
OR (27302)
  (( segid "BrD " and resid 56   and name HG  ))
  (( segid "BrD " and resid 77   and name HB1 ))
ASSI (27332)
  (( segid "BrD " and resid 56   and name HG  ))
  (  segid "BrD " and resid 81   and name HG2%)
    3.600      3.200      1.900 peak 27332 weight  0.10000E+01 volume  0.35670E+02 ppm1      2.338 ppm2      0.758
OR (27332)
  (( segid "BrD " and resid 22   and name HG  ))
  (  segid "BrD " and resid 78   and name HD1%)
ASSI (27462)
  (  segid "BrD " and resid 22   and name HD1%)
  (( segid "BrD " and resid 25   and name HB  ))
    3.800      3.600      1.700 peak 27462 weight  0.10000E+01 volume  0.26281E+02 ppm1      1.648 ppm2      2.995
OR (27462)
  (  segid "BrD " and resid 22   and name HD1%)
  (( segid "BrD " and resid 61   and name HG1 ))
OR (27462)
  (  segid "BrD " and resid 22   and name HD1%)
  (( segid "BrD " and resid 74   and name HB2 ))
ASSI (27482)
  (  segid "BrD " and resid 22   and name HD2%)
  (( segid "BrD " and resid 26   and name HA  ))
    3.200      2.600      2.300 peak 27482 weight  0.10000E+01 volume  0.77977E+02 ppm1      1.599 ppm2      4.492
OR (27482)
  (  segid "BrD " and resid 22   and name HD2%)
  (( segid "BrD " and resid 58   and name HA  ))
ASSI (27502)
  (  segid "BrD " and resid 22   and name HD2%)
  (( segid "BrD " and resid 59   and name HA  ))
    3.200      2.600      2.300 peak 27502 weight  0.10000E+01 volume  0.74913E+02 ppm1      1.599 ppm2      4.901
OR (27502)
  (  segid "BrD " and resid 22   and name HD2%)
  (( segid "BrD " and resid 35   and name HA  ))
OR (27502)
  (  segid "BrD " and resid 22   and name HD2%)
  (( segid "BrD " and resid 20   and name HA  ))
ASSI (27542)
  (  segid "BrD " and resid 22   and name HD2%)
  (( segid "BrD " and resid 56   and name HB2 ))
    4.000      4.000      1.500 peak 27542 weight  0.10000E+01 volume  0.19846E+02 ppm1      1.599 ppm2      2.011
OR (27542)
  (  segid "BrD " and resid 22   and name HD2%)
  (( segid "BrD " and resid 61   and name HB  ))
ASSI (27562)
  (  segid "BrD " and resid 22   and name HD1%)
  (( segid "BrD " and resid 64   and name HA  ))
    3.300      2.700      2.200 peak 27562 weight  0.10000E+01 volume  0.62753E+02 ppm1      1.645 ppm2      4.911
OR (27562)
  (  segid "BrD " and resid 22   and name HD1%)
  (( segid "BrD " and resid 59   and name HA  ))
ASSI (27592)
  (( segid "BrD " and resid 110  and name HG12))
  (  segid "BrD " and resid 115  and name HD1%)
    3.300      2.700      2.200 peak 27592 weight  0.10000E+01 volume  0.61111E+02 ppm1      1.646 ppm2      1.321
OR (27592)
  (( segid "BrD " and resid 110  and name HG12))
  (( segid "BrD " and resid 78   and name HB1 ))
OR (27592)
  (  segid "BrD " and resid 22   and name HD1%)
  (  segid "BrD " and resid 102  and name HD2%)
OR (27592)
  (( segid "BrD " and resid 110  and name HG12))
  (  segid "BrD " and resid 102  and name HD2%)
ASSI (27622)
  (  segid "BrD " and resid 73   and name HD2%)
  (( segid "BrD " and resid 74   and name HA  ))
    3.000      2.200      2.200 peak 27622 weight  0.10000E+01 volume  0.10007E+03 ppm1      1.500 ppm2      4.363
OR (27622)
  (  segid "BrD " and resid 73   and name HD2%)
  (( segid "BrD " and resid 70   and name HB2 ))
ASSI (27832)
  (( segid "BrD " and resid 78   and name HA  ))
  (( segid "BrD " and resid 82   and name HZ  ))
    3.500      3.100      2.000 peak 27832 weight  0.10000E+01 volume  0.44344E+02 ppm1      3.966 ppm2      7.023
OR (27832)
  (( segid "BrD " and resid 78   and name HA  ))
  (  segid "BrD " and resid 74   and name HD% )
ASSI (27862)
  (( segid "BrD " and resid 78   and name HB2 ))
  (( segid "BrD " and resid 116  and name HG12))
    4.700      4.700      0.800 peak 27852 weight  0.10000E+01 volume  0.74355E+01 ppm1      1.056 ppm2      1.531
OR (27852)
  (( segid "BrD " and resid 78   and name HB2 ))
  (  segid "BrD " and resid 56   and name HD1%)
ASSI (27862)
  (( segid "BrD " and resid 78   and name HB2 ))
  (( segid "BrD " and resid 110  and name HG12))
    3.700      3.400      1.800 peak 27862 weight  0.10000E+01 volume  0.33112E+02 ppm1      1.054 ppm2      1.629
OR (27862)
  (( segid "BrD " and resid 78   and name HB2 ))
  (  segid "BrD " and resid 21   and name HG2%)
OR (27862)
  (( segid "BrD " and resid 78   and name HB2 ))
  (  segid "BrD " and resid 22   and name HD2%)
OR (27862)
  (( segid "BrD " and resid 78   and name HB2 ))
  (( segid "BrD " and resid 21   and name HG12))
ASSI (27962)
  (  segid "BrD " and resid 78   and name HD1%)
  (  segid "BrD " and resid 74   and name HD% )
    2.200      2.200      2.300 peak 27962 weight  0.10000E+01 volume  0.80433E+03 ppm1      0.761 ppm2      7.031
OR (27962)
  (  segid "BrD " and resid 78   and name HD1%)
  (  segid "BrD " and resid 82   and name HE% )
ASSI (28022)
  (  segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 22   and name HA  ))
    1.100      2.400      2.400 peak 28022 weight  0.10000E+01 volume  0.92248E+02 ppm1      0.662 ppm2      4.727
OR (28022)
  (  segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 82   and name HA  ))
ASSI (28042)
  (  segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 56   and name HA  ))
    3.600      3.200      1.900 peak 28042 weight  0.10000E+01 volume  0.33967E+02 ppm1      0.662 ppm2      4.631
OR (28042)
  (  segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 76   and name HA  ))
OR (28042)
  (  segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 80   and name HA  ))
OR (28042)
  (  segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 104  and name HA  ))
OR (28042)
  (  segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 20   and name HB1 ))
OR (28042)
  (  segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 109  and name HA  ))
OR (28042)
  (  segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 14   and name HA  ))
OR (28042)
  (  segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 71   and name HA  ))
OR (28042)
  (  segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 15   and name HA  ))
ASSI (28052)
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   ( segid "BrD " and resid 78   and name HD1%)
   (( segid "BrD " and resid 56   and name HA  ))
      3.800      3.600      1.700 peak 28052 weight  0.10000E+01 volume  0.28600E+02 ppm1      0.761 ppm2      4.631
OR (28052)
   ( segid "BrD " and resid 78   and name HD1%)
   (( segid "BrD " and resid 76   and name HA  ))
OR (28052)
   ( segid "BrD " and resid 78   and name HD1%)
   (( segid "BrD " and resid 80   and name HA  ))
OR (28052)
   ( segid "BrD " and resid 78   and name HD1%)
   (( segid "BrD " and resid 60   and name HB2 ))
ASSI (28072)
   ( segid "BrD " and resid 78   and name HD1%)
   (( segid "BrD " and resid 79   and name HA  ))
      3.400      2.900      2.100 peak 28072 weight  0.10000E+01 volume  0.48389E+02 ppm1      0.761 ppm2      4.428
OR (28072)
   ( segid "BrD " and resid 78   and name HD1%)
   (( segid "BrD " and resid 25   and name HA  ))
OR (28072)
   ( segid "BrD " and resid 78   and name HD1%)
   (( segid "BrD " and resid 107  and name HA  ))
OR (28072)
   ( segid "BrD " and resid 78   and name HD1%)
   (( segid "BrD " and resid 99   and name HA  ))
ASSI (28082)
   ( segid "BrD " and resid 78   and name HD2%)
   (( segid "BrD " and resid 106  and name HA  ))
      3.000      2.200      2.200 peak 28082 weight  0.10000E+01 volume  0.10774E+03 ppm1      0.662 ppm2      4.525
OR (28082)
   ( segid "BrD " and resid 78   and name HD2%)
   (( segid "BrD " and resid 75   and name HA  ))
ASSI (28092)
   ( segid "BrD " and resid 78   and name HD2%)
   (( segid "BrD " and resid 79   and name HA  ))
      2.900      2.100      2.100 peak 28092 weight  0.10000E+01 volume  0.12398E+03 ppm1      0.662 ppm2      4.427
OR (28092)
   ( segid "BrD " and resid 78   and name HD2%)
   (( segid "BrD " and resid 107  and name HA  ))
ASSI (28112)
   ( segid "BrD " and resid 78   and name HD1%)
   (( segid "BrD " and resid 106  and name HB2 ))
      3.200      2.600      2.300 peak 28112 weight  0.10000E+01 volume  0.76864E+02 ppm1      0.760 ppm2      3.711
OR (28112)
   ( segid "BrD " and resid 78   and name HD1%)
   (( segid "BrD " and resid 81   and name HA  ))
ASSI (28142)
   ( segid "BrD " and resid 78   and name HD2%)
   (( segid "BrD " and resid 25   and name HB  ))
      3.900      3.800      1.600 peak 28142 weight  0.10000E+01 volume  0.22598E+02 ppm1      0.662 ppm2      3.005
OR (28142)
   ( segid "BrD " and resid 78   and name HD2%)
   (( segid "BrD " and resid 79   and name HG1 ))
OR (28142)
   ( segid "BrD " and resid 78   and name HD2%)
   (( segid "BrD " and resid 74   and name HB2 ))
ASSI (28152)
   ( segid "BrD " and resid 78   and name HD2%)
   (( segid "BrD " and resid 21   and name HG11))
      3.600      3.200      1.900 peak 28152 weight  0.10000E+01 volume  0.38156E+02 ppm1      0.662 ppm2      2.347
OR (28152)
   ( segid "BrD " and resid 78   and name HD2%)
   (( segid "BrD " and resid 56   and name HG  ))
OR (28152)
   ( segid "BrD " and resid 78   and name HD2%)
   (( segid "BrD " and resid 22   and name HG  ))
ASSI (28162)
   ( segid "BrD " and resid 78   and name HD2%)
   ( segid "BrD " and resid 75   and name HE% )
      4.300      4.300      1.200 peak 28162 weight  0.10000E+01 volume  0.12997E+02 ppm1      0.662 ppm2      2.670
OR (28162)
   ( segid "BrD " and resid 78   and name HD2%)
   (( segid "BrD " and resid 79   and name HB2 ))
OR (28162)
   ( segid "BrD " and resid 78   and name HD2%)
   (( segid "BrD " and resid 22   and name HB1 ))
ASSI (28172)
   ( segid "BrD " and resid 78   and name HD1%)
   (( segid "BrD " and resid 74   and name HB2 ))
      3.800      3.600      1.700 peak 28172 weight  0.10000E+01 volume  0.27394E+02 ppm1      0.760 ppm2      3.003
OR (28172)
   ( segid "BrD " and resid 78   and name HD1%)
   (( segid "BrD " and resid 25   and name HB  ))
ASSI (28302)
   ( segid "BrD " and resid 56   and name HD2%)
   (( segid "BrD " and resid 35   and name HA  ))
      2.600      1.700      1.700 peak 28302 weight  0.10000E+01 volume  0.27298E+03 ppm1      1.254 ppm2      4.907
OR (28302)
   ( segid "BrD " and resid 56   and name HD2%)
   (( segid "BrD " and resid 59   and name HA  ))
ASSI (28332)
   ( segid "BrD " and resid 56   and name HD2%)
   (( segid "BrD " and resid 25   and name HA  ))
      5.000      5.000      0.500 peak 28332 weight  0.10000E+01 volume  0.51532E+01 ppm1      1.253 ppm2      4.441
OR (28332)
   ( segid "BrD " and resid 56   and name HD2%)
   (( segid "BrD " and resid 58   and name HA  ))
ASSI (28482)
   (( segid "BrD " and resid 56   and name HB2 ))
   ( segid "BrD " and resid 81   and name HG2%)
      3.700      3.400      1.800 peak 28482 weight  0.10000E+01 volume  0.33282E+02 ppm1      1.993 ppm2      0.766
OR (28482)
   (( segid "BrD " and resid 102  and name HB1 ))
   ( segid "BrD " and resid 81   and name HG2%)
ASSI (28552)
   (( segid "BrD " and resid 102  and name HG  ))
   (( segid "BrD " and resid 25   and name HA  ))
      4.000      4.000      1.500 peak 28552 weight  0.10000E+01 volume  0.18876E+02 ppm1      2.141 ppm2      4.445
OR (28552)
   (( segid "BrD " and resid 102  and name HG  ))
   (( segid "BrD " and resid 99   and name HA  ))
OR (28552)
   (( segid "BrD " and resid 97   and name HG2 ))
   (( segid "BrD " and resid 96   and name HA  ))
ASSI (28592)
   ( segid "BrD " and resid 102  and name HD2%)
   (( segid "BrD " and resid 34   and name HZ  ))
      3.700      3.400      1.800 peak 28592 weight  0.10000E+01 volume  0.30371E+02 ppm1      1.303 ppm2      7.899
OR (28592)
   ( segid "BrD " and resid 102  and name HD2%)
   ( segid "BrD " and resid 107  and name HE% )
ASSI (28602)
   ( segid "BrD " and resid 102  and name HD2%)
   ( segid "BrD " and resid 34   and name HE% )
      2.000      2.000      2.500 peak 28602 weight  0.10000E+01 volume  0.10851E+04 ppm1      1.303 ppm2      7.771
OR (28602)
   ( segid "BrD " and resid 102  and name HD2%)
   ( segid "BrD " and resid 105  and name HD% )
ASSI (28682)
   ( segid "BrD " and resid 102  and name HD1%)
   (( segid "BrD " and resid 28   and name HA  ))
      4.000      4.000      1.500 peak 28682 weight  0.10000E+01 volume  0.20825E+02 ppm1      1.303 ppm2      4.581
OR (28682)
   ( segid "BrD " and resid 102  and name HD1%)
   (( segid "BrD " and resid 106  and name HA  ))
ASSI (28692)
   ( segid "BrD " and resid 102  and name HD1%)
   (( segid "BrD " and resid 30   and name HB2 ))
      2.700      1.800      1.800 peak 28692 weight  0.10000E+01 volume  0.20830E+03 ppm1      1.303 ppm2      4.526
OR (28692)
   ( segid "BrD " and resid 102  and name HD1%)
   (( segid "BrD " and resid 28   and name HA  ))
ASSI (28772)
   ( segid "BrD " and resid 102  and name HD2%)
   ( segid "BrD " and resid 78   and name HD1%)
      3.500      3.100      2.000 peak 28772 weight  0.10000E+01 volume  0.44195E+02 ppm1      1.304 ppm2      0.760
OR (28772)
   ( segid "BrD " and resid 102  and name HD2%)
   ( segid "BrD " and resid 81   and name HG2%)
ASSI (28862)
   (( segid "BrD " and resid 115  and name HB1 ))
   (( segid "BrD " and resid 110  and name HG11))
      3.300      2.700      2.200 peak 28862 weight  0.10000E+01 volume  0.61541E+02 ppm1      2.190 ppm2      1.742
OR (28862)
   (( segid "BrD " and resid 115  and name HB1 ))
   ( segid "BrD " and resid 17   and name HG2%)
ASSI (28952)
   ( segid "BrD " and resid 56   and name HD1%)
   (( segid "BrD " and resid 31   and name HA  ))
      3.100      2.400      2.400 peak 28952 weight  0.10000E+01 volume  0.92579E+02 ppm1      1.548 ppm2      4.984
OR (28952)
   ( segid "BrD " and resid 56   and name HD1%)
   (( segid "BrD " and resid 60   and name HB1 ))
ASSI (29002)
   ( segid "BrD " and resid 59   and name HE% )
   ( segid "BrD " and resid 76   and name HB% )
      3.500      3.100      2.000 peak 29002 weight  0.10000E+01 volume  0.43704E+02 ppm1      1.848 ppm2      2.108
OR (29002)
   ( segid "BrD " and resid 59   and name HE% )
   (( segid "BrD " and resid 18   and name HB1 ))
OR (29002)
   ( segid "BrD " and resid 59   and name HE% )
   (( segid "BrD " and resid 102  and name HG  ))
ASSI (29022)
   ( segid "BrD " and resid 59   and name HE% )
   (( segid "BrD " and resid 22   and name HB2 ))
      3.400      2.800      2.100 peak 29022 weight  0.10000E+01 volume  0.52140E+02 ppm1      1.848 ppm2      2.292
OR (29022)
   ( segid "BrD " and resid 59   and name HE% )
   (( segid "BrD " and resid 18   and name HG  ))
OR (29022)
   ( segid "BrD " and resid 69   and name HE% )
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   ( segid "BrD " and resid 31   and name HB% )
ASSI {29032}
   ( segid "BrD " and resid 59   and name HE% )
   (( segid "BrD " and resid 56   and name HG  ))
     3.700      3.400      1.800 peak 29032 weight  0.10000E+01 volume  0.29631E+02 ppm1      1.848 ppm2      2.361
OR {29032}
   ( segid "BrD " and resid 59   and name HE% )
   (( segid "BrD " and resid 22   and name HG  ))
OR {29032}
   ( segid "BrD " and resid 59   and name HE% )
   (( segid "BrD " and resid 73   and name HG  ))
OR {29032}
   ( segid "BrD " and resid 59   and name HE% )
   (( segid "BrD " and resid 21   and name HG11))
ASSI {29072}
   ( segid "BrD " and resid 59   and name HE% )
   (( segid "BrD " and resid 22   and name HA  ))
     4.200      4.200      1.300 peak 29072 weight  0.10000E+01 volume  0.14615E+02 ppm1      1.848 ppm2      4.719
OR {29072}
   ( segid "BrD " and resid 59   and name HE% )
   (( segid "BrD " and resid 58   and name HB  ))
OR {29072}
   ( segid "BrD " and resid 59   and name HE% )
   (( segid "BrD " and resid 69   and name HA  ))
OR {29072}
   ( segid "BrD " and resid 59   and name HE% )
   (( segid "BrD " and resid 53   and name HA  ))
ASSI {29152}
   ( segid "BrD " and resid 59   and name HE% )
   ( segid "BrD " and resid 73   and name HD2%)
     3.600      3.200      1.900 peak 29152 weight  0.10000E+01 volume  0.38252E+02 ppm1      1.848 ppm2      1.462
OR {29152}
   ( segid "BrD " and resid 59   and name HE% )
   ( segid "BrD " and resid 63   and name HD2%)
OR {29152}
   ( segid "BrD " and resid 59   and name HE% )
   (( segid "BrD " and resid 62   and name HG2 ))
ASSI {29192}
   ( segid "BrD " and resid 54   and name HE% )
   (( segid "BrD " and resid 60   and name HB1 ))
     3.200      2.600      2.300 peak 29192 weight  0.10000E+01 volume  0.76364E+02 ppm1      2.536 ppm2      4.964
OR {29192}
   ( segid "BrD " and resid 54   and name HE% )
   (( segid "BrD " and resid 77   and name HA  ))
ASSI {29202}
   ( segid "BrD " and resid 54   and name HE% )
   (( segid "BrD " and resid 55   and name HB1 ))
     3.700      3.400      1.800 peak 29202 weight  0.10000E+01 volume  0.30281E+02 ppm1      2.535 ppm2      2.955
OR {29202}
   ( segid "BrD " and resid 54   and name HE% )
   (( segid "BrD " and resid 37   and name HB1 ))
ASSI {29252}
   ( segid "BrD " and resid 54   and name HE% )
   ( segid "BrD " and resid 35   and name HE% )
     2.500      2.500      2.000 peak 29252 weight  0.10000E+01 volume  0.29954E+03 ppm1      2.535 ppm2      2.801
OR {29252}
   ( segid "BrD " and resid 54   and name HE% )
   (( segid "BrD " and resid 53   and name HB1 ))
OR {29252}
   ( segid "BrD " and resid 54   and name HE% )
   (( segid "BrD " and resid 61   and name HG2 ))
OR {29252}
   ( segid "BrD " and resid 54   and name HE% )
   (( segid "BrD " and resid 36   and name HG1 ))
ASSI {29262}
   ( segid "BrD " and resid 54   and name HE% )
   (( segid "BrD " and resid 37   and name HG1 ))
     2.600      1.700      1.700 peak 29262 weight  0.10000E+01 volume  0.23100E+03 ppm1      2.535 ppm2      2.722
OR {29262}
   ( segid "BrD " and resid 54   and name HE% )
   (( segid "BrD " and resid 59   and name HB1 ))
ASSI {29582}
   (( segid "BrD " and resid 79   and name HA  ))
   (( segid "BrD " and resid 116  and name HG11))
     4.100      4.100      1.400 peak 29582 weight  0.10000E+01 volume  0.16991E+02 ppm1      4.409 ppm2      1.897
OR {29582}
   (( segid "BrD " and resid 79   and name HA  ))
   (( segid "BrD " and resid 103  and name HB2 ))
ASSI {29682}
   (( segid "BrD " and resid 108  and name HA  ))
   (( segid "BrD " and resid 111  and name HG1 ))
     4.100      4.100      1.400 peak 29682 weight  0.10000E+01 volume  0.16470E+02 ppm1      4.804 ppm2      2.003
OR {29682}
   (( segid "BrD " and resid 108  and name HA  ))
   (( segid "BrD " and resid 109  and name HD1 ))
ASSI {29702}
   (( segid "BrD " and resid 15   and name HA  ))
   (( segid "BrD " and resid 19   and name HB2 ))
     2.800      2.000      2.000 peak 29702 weight  0.10000E+01 volume  0.16053E+03 ppm1      4.607 ppm2      1.986
OR {29702}
   (( segid "BrD " and resid 108  and name HB1 ))
   (( segid "BrD " and resid 109  and name HD1 ))
OR {29702}
   (( segid "BrD " and resid 60   and name HB2 ))
   (( segid "BrD " and resid 56   and name HB2 ))
ASSI {29712}
   (( segid "BrD " and resid 15   and name HA  ))
   (( segid "BrD " and resid 18   and name HB1 ))
     3.100      2.400      2.400 peak 29712 weight  0.10000E+01 volume  0.92305E+02 ppm1      4.607 ppm2      2.182
OR {29712}
   (( segid "BrD " and resid 60   and name HB2 ))
   (( segid "BrD " and resid 64   and name HG1 ))
ASSI {29722}
   (( segid "BrD " and resid 15   and name HA  ))
   ( segid "BrD " and resid 14   and name HD2%)
     3.900      3.800      1.600 peak 29722 weight  0.10000E+01 volume  0.22638E+02 ppm1      4.607 ppm2      1.417
OR {29722}
   (( segid "BrD " and resid 15   and name HA  ))
   ( segid "BrD " and resid 69   and name HG2%)
ASSI {29732}
   (( segid "BrD " and resid 10   and name HA  ))
   (( segid "BrD " and resid 98   and name HA  ))
     2.600      1.700      1.700 peak 29732 weight  0.10000E+01 volume  0.26724E+03 ppm1      5.445 ppm2      4.810
OR {29732}
   (( segid "BrD " and resid 10   and name HA  ))
   (( segid "BrD " and resid 29   and name HA  ))
ASSI {30592}
   (( segid "BrD " and resid 109  and name HB1 ))
   ( segid "BrD " and resid 21   and name HD1%)
     3.700      3.400      1.800 peak 30592 weight  0.10000E+01 volume  0.31262E+02 ppm1      2.334 ppm2      1.222
OR {30592}
   (( segid "BrD " and resid 109  and name HB1 ))
   ( segid "BrD " and resid 110  and name HG2%)
ASSI {30672}
   (( segid "BrD " and resid 109  and name HB2 ))
   (( segid "BrD " and resid 110  and name HA  ))
     3.600      3.200      1.900 peak 30672 weight  0.10000E+01 volume  0.39278E+02 ppm1      2.141 ppm2      4.378
OR {30672}
   (( segid "BrD " and resid 109  and name HB2 ))
   (( segid "BrD " and resid 107  and name HA  ))
ASSI {30952}
   (( segid "BrD " and resid 75   and name HA  ))
   (( segid "BrD " and resid 78   and name HG  ))
     3.800      3.600      1.700 peak 30952 weight  0.10000E+01 volume  0.28077E+02 ppm1      4.509 ppm2      1.260
OR {30952}
   (( segid "BrD " and resid 26   and name HA  ))
   ( segid "BrD " and resid 56   and name HD2%)
ASSI {   83}
   ( segid "BrD " and resid 46   and name HD% )
   (( segid "BrD " and resid 47   and name HA  ))
     2.300      2.300      2.200 peak    83 weight  0.10000E+01 volume  0.20163E+03 ppm1      5.758 ppm2      4.693
OR {   83}
   ( segid "BrD " and resid 46   and name HD% )
   (( segid "BrD " and resid 53   and name HA  ))
ASSI {  533}
   ( segid "BrD " and resid 47   and name HE% )
   (( segid "BrD " and resid 38   and name HB  ))
     3.200      2.600      2.300 peak   533 weight  0.10000E+01 volume  0.34245E+02 ppm1      7.246 ppm2      1.776
OR {  533}
   ( segid "BrD " and resid 47   and name HE% )
   (( segid "BrD " and resid 50   and name HB  ))
ASSI {  643}
   ( segid "BrD " and resid 74   and name HD% )
   (( segid "BrD " and resid 71   and name HA  ))
     3.100      2.400      2.400 peak   643 weight  0.10000E+01 volume  0.35398E+02 ppm1      7.012 ppm2      4.622
OR {  643}
   ( segid "BrD " and resid 74   and name HD% )
   (( segid "BrD " and resid 15   and name HA  ))
OR {  643}
   ( segid "BrD " and resid 74   and name HD% )
   (( segid "BrD " and resid 76   and name HA  ))
OR {  643}
   ( segid "BrD " and resid 74   and name HD% )
   (( segid "BrD " and resid 56   and name HA  ))
OR {  643}
   ( segid "BrD " and resid 74   and name HD% )
   (( segid "BrD " and resid 72   and name HA  ))
OR {  643}
   ( segid "BrD " and resid 74   and name HD% )
   (( segid "BrD " and resid 14   and name HA  ))
ASSI { 1143}
   ( segid "BrD " and resid 105  and name HD% )
   ( segid "BrD " and resid 101  and name HG2%)
     3.100      2.400      2.400 peak  1143 weight  0.10000E+01 volume  0.36890E+02 ppm1      7.758 ppm2      1.631
OR { 1143}
   ( segid "BrD " and resid 105  and name HD% )
   ( segid "BrD " and resid 21   and name HG2%)
ASSI { 1393}
   ( segid "BrD " and resid 96   and name HD% )
   (( segid "BrD " and resid 86   and name HA  ))
     2.200      2.200      2.300 peak  1393 weight  0.10000E+01 volume  0.26898E+03 ppm1      7.711 ppm2      4.810
OR { 1393}
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   (  segid "BrD " and resid 96   and name HD% )
   (( segid "BrD " and resid 92   and name HA  ))
ASSI [ 1763]
   (  segid "BrD " and resid 106  and name HE% )
   (( segid "BrD " and resid 107  and name HA  ))
      3.400      2.900      2.100 peak  1763 weight  0.10000E+01 volume  0.21871E+02 ppm1      7.617 ppm2      4.431
OR [ 1763]
   (  segid "BrD " and resid 106  and name HE% )
   (( segid "BrD " and resid 79   and name HA  ))
OR [ 1763]
   (  segid "BrD " and resid 106  and name HE% )
   (( segid "BrD " and resid 110  and name HA  ))
ASSI [ 1783]
   (  segid "BrD " and resid 106  and name HE% )
   (  segid "BrD " and resid 74   and name HD% )
      3.700      3.400      1.800 peak  1783 weight  0.10000E+01 volume  0.13872E+02 ppm1      7.617 ppm2      7.027
OR [ 1783]
   (  segid "BrD " and resid 106  and name HE% )
   (  segid "BrD " and resid 82   and name HE% )
OR [ 1783]
   (  segid "BrD " and resid 106  and name HE% )
   (( segid "BrD " and resid 62   and name HZ  ))
ASSI [ 1813]
   (  segid "BrD " and resid 95   and name HD% )
   (( segid "BrD " and resid 94   and name HA  ))
      3.300      2.700      2.200 peak  1813 weight  0.10000E+01 volume  0.28141E+02 ppm1      7.478 ppm2      4.810
OR [ 1813]
   (  segid "BrD " and resid 95   and name HD% )
   (( segid "BrD " and resid 86   and name HA  ))
ASSI [ 1893]
   (  segid "BrD " and resid 96   and name HE% )
   (( segid "BrD " and resid 96   and name HA  ))
      3.600      3.200      1.900 peak  1893 weight  0.10000E+01 volume  0.14793E+02 ppm1      7.618 ppm2      4.387
OR [ 1893]
   (  segid "BrD " and resid 95   and name HE% )
   (( segid "BrD " and resid 33   and name HA  ))
ASSI [ 2063]
   (( segid "BrD " and resid 32   and name HZ3 ))
   (( segid "BrD " and resid 32   and name HA  ))
      5.500      5.500      0.000 peak  2063 weight  0.10000E+01 volume  0.11153E-03 ppm1      7.804 ppm2      4.971
OR [ 2063]
   (( segid "BrD " and resid 32   and name HZ3 ))
   (( segid "BrD " and resid 93   and name HB1 ))
OR [ 2063]
   (( segid "BrD " and resid 32   and name HZ3 ))
   (( segid "BrD " and resid 85   and name HA  ))
ASSI [   24]
   (  segid "BrD " and resid 46   and name HE% )
   (( segid "BrD " and resid 50   and name HB  ))
      3.600      3.200      1.900 peak    24 weight  0.10000E+01 volume  0.55296E+02 ppm1      6.687 ppm2      1.777
OR [   24]
   (  segid "BrD " and resid 46   and name HE% )
   (( segid "BrD " and resid 38   and name HB  ))
ASSI [   94]
   (  segid "BrD " and resid 82   and name HD% )
   (( segid "BrD " and resid 79   and name HA  ))
      2.200      1.200      1.200 peak    94 weight  0.10000E+01 volume  0.10359E+04 ppm1      7.266 ppm2      4.424
OR [   94]
   (  segid "BrD " and resid 82   and name HD% )
   (( segid "BrD " and resid 99   and name HA  ))
ASSI [  104]
   (  segid "BrD " and resid 47   and name HE% )
   (( segid "BrD " and resid 53   and name HG2 ))
      2.500      1.600      1.600 peak   104 weight  0.10000E+01 volume  0.51564E+03 ppm1      7.270 ppm2      2.504
OR [  104]
   (  segid "BrD " and resid 82   and name HD% )
   (( segid "BrD " and resid 103  and name HG2 ))
ASSI [  124]
   (  segid "BrD " and resid 47   and name HD% )
   (( segid "BrD " and resid 50   and name HG12))
      3.600      3.200      1.900 peak   124 weight  0.10000E+01 volume  0.55730E+02 ppm1      7.970 ppm2      0.780
OR [  124]
   (  segid "BrD " and resid 47   and name HD% )
   (  segid "BrD " and resid 38   and name HG2%)
ASSI [  134]
   (  segid "BrD " and resid 47   and name HD% )
   (( segid "BrD " and resid 53   and name HD2 ))
      2.900      2.100      2.100 peak   134 weight  0.10000E+01 volume  0.18431E+03 ppm1      7.970 ppm2      4.007
OR [  134]
   (( segid "BrD " and resid 32   and name HZ2 ))
   (( segid "BrD " and resid 98   and name HB1 ))
ASSI [  554]
   (( segid "BrD " and resid 28   and name HE1 ))
   (( segid "BrD " and resid 30   and name HB2 ))
      2.900      2.100      2.100 peak   554 weight  0.10000E+01 volume  0.21924E+03 ppm1      8.156 ppm2      4.538
OR [  554]
   (( segid "BrD " and resid 28   and name HE1 ))
   (( segid "BrD " and resid 28   and name HA  ))
ASSI [  574]
   (  segid "BrD " and resid 68   and name HE% )
   (( segid "BrD " and resid 59   and name HA  ))
      3.200      2.600      2.300 peak   574 weight  0.10000E+01 volume  0.10500E+03 ppm1      7.921 ppm2      4.930
OR [  574]
   (( segid "BrD " and resid 32   and name HE3 ))
   (( segid "BrD " and resid 32   and name HA  ))
ASSI [  604]
   (( segid "BrD " and resid 107  and name HZ  ))
   (( segid "BrD " and resid 83   and name HB  ))
      3.500      3.100      2.000 peak   604 weight  0.10000E+01 volume  0.65660E+02 ppm1      8.063 ppm2      4.784
OR [  604]
   (( segid "BrD " and resid 107  and name HZ  ))
   (( segid "BrD " and resid 82   and name HA  ))
ASSI [  614]
   (( segid "BrD " and resid 107  and name HZ  ))
   (( segid "BrD " and resid 80   and name HA  ))
      3.300      2.700      2.200 peak   614 weight  0.10000E+01 volume  0.96219E+02 ppm1      8.062 ppm2      4.673
OR [  614]
   (( segid "BrD " and resid 107  and name HZ  ))
   (( segid "BrD " and resid 118  and name HA  ))
OR [  614]
   (( segid "BrD " and resid 107  and name HZ  ))
   (( segid "BrD " and resid 76   and name HA  ))
ASSI [  704]
   (( segid "BrD " and resid 107  and name HZ  ))
   (( segid "BrD " and resid 79   and name HB1 ))
      2.600      2.000      2.000 peak   704 weight  0.10000E+01 volume  0.35291E+03 ppm1      8.009 ppm2      2.755
OR [  704]
   (( segid "BrD " and resid 32   and name HZ2 ))
   (( segid "BrD " and resid 94   and name HB1 ))
ASSI [  794]
   (( segid "BrD " and resid 32   and name HE3 ))
   (( segid "BrD " and resid 32   and name HB2 ))
      2.600      1.700      1.700 peak   794 weight  0.10000E+01 volume  0.39954E+03 ppm1      7.960 ppm2      4.212
OR [  794]
   (  segid "BrD " and resid 47   and name HD% )
   (( segid "BrD " and resid 53   and name HD1 ))
ASSI [  964]
   (( segid "BrD " and resid 34   and name HZ  ))
   (( segid "BrD " and resid 28   and name HD2 ))
      4.200      4.200      1.300 peak   964 weight  0.10000E+01 volume  0.22395E+02 ppm1      7.928 ppm2      5.579
OR [  964]
   (( segid "BrD " and resid 34   and name HZ  ))
   (( segid "BrD " and resid 34   and name HA  ))
ASSI [  974]
   (( segid "BrD " and resid 34   and name HZ  ))
   (( segid "BrD " and resid 98   and name HA  ))
      3.800      3.600      1.700 peak   974 weight  0.10000E+01 volume  0.41681E+02 ppm1      7.929 ppm2      4.791
OR [  974]
   (( segid "BrD " and resid 34   and name HZ  ))
   (( segid "BrD " and resid 82   and name HA  ))
ASSI [ 1044]
   (  segid "BrD " and resid 107  and name HE% )
   (( segid "BrD " and resid 79   and name HA  ))
      2.300      1.300      1.300 peak  1044 weight  0.10000E+01 volume  0.88364E+03 ppm1      7.921 ppm2      4.440
OR [ 1044]
   (( segid "BrD " and resid 34   and name HZ  ))
   (( segid "BrD " and resid 99   and name HA  ))
ASSI [ 1074]
   (( segid "BrD " and resid 34   and name HZ  ))
   (  segid "BrD " and resid 102  and name HD1%)
      2.900      2.100      2.100 peak  1074 weight  0.10000E+01 volume  0.20962E+03 ppm1      7.924 ppm2      1.333
OR [ 1074]
   (  segid "BrD " and resid 107  and name HE% )
   (( segid "BrD " and resid 78   and name HB1 ))
ASSI [ 1084]
   (( segid "BrD " and resid 34   and name HZ  ))
   (( segid "BrD " and resid 98   and name HA  ))
      4.000      4.000      1.500 peak  1084 weight  0.10000E+01 volume  0.28521E+02 ppm1      7.913 ppm2      4.791
OR [ 1084]
   (( segid "BrD " and resid 34   and name HZ  ))
   (( segid "BrD " and resid 82   and name HA  ))
OR [ 1084]
   (  segid "BrD " and resid 68   and name HE% )
   (( segid "BrD " and resid 73   and name HA  ))
ASSI [ 1094]
   (  segid "BrD " and resid 107  and name HE% )
   (( segid "BrD " and resid 118  and name HA  ))
      3.200      2.600      2.300 peak  1094 weight  0.10000E+01 volume  0.10760E+03 ppm1      7.918 ppm2      4.683
OR [ 1094]
   (  segid "BrD " and resid 107  and name HE% )
   (( segid "BrD " and resid 76   and name HA  ))
OR [ 1094]
   (  segid "BrD " and resid 68   and name HE% )
   (( segid "BrD " and resid 58   and name HB  ))
OR [ 1094]
   (  segid "BrD " and resid 68   and name HE% )
   (( segid "BrD " and resid 67   and name HA  ))
OR [ 1094]
   (  segid "BrD " and resid 107  and name HE% )
   (( segid "BrD " and resid 104  and name HA  ))
OR [ 1094]
   (  segid "BrD " and resid 107  and name HE% )
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   (( segid "BrD " and resid 80   and name HA  ))
OR ( 1094)
   (  segid "BrD " and resid 68   and name HE% )
   (( segid "BrD " and resid 69   and name HA  ))
ASSI ( 1104)
   (( segid "BrD " and resid 34   and name HZ  ))
   (  segid "BrD " and resid 99   and name HB% )
      2.400      1.400      1.400 peak  1104 weight  0.10000E+01 volume  0.63603E+03 ppm1      7.907 ppm2      2.212
OR ( 1104)
   (( segid "BrD " and resid 34   and name HZ  ))
   (( segid "BrD " and resid 33   and name HD2 ))
ASSI ( 1114)
   (  segid "BrD " and resid 68   and name HE% )
   (  segid "BrD " and resid 68   and name HD% )
      2.100      1.100      1.100 peak  1114 weight  0.10000E+01 volume  0.15242E+04 ppm1      7.904 ppm2      7.776
OR ( 1114)
   (  segid "BrD " and resid 107  and name HE% )
   (  segid "BrD " and resid 107  and name HD% )
OR ( 1114)
   (( segid "BrD " and resid 34   and name HZ  ))
   (  segid "BrD " and resid 34   and name HE% )
ASSI ( 1124)
   (( segid "BrD " and resid 34   and name HZ  ))
   (( segid "BrD " and resid 98   and name HB2 ))
      2.500      1.600      1.600 peak  1124 weight  0.10000E+01 volume  0.54441E+03 ppm1      7.898 ppm2      3.659
OR ( 1124)
   (  segid "BrD " and resid 107  and name HE% )
   (( segid "BrD " and resid 82   and name HB1 ))
OR ( 1124)
   (  segid "BrD " and resid 68   and name HE% )
   (( segid "BrD " and resid 68   and name HB1 ))
ASSI ( 1134)
   (  segid "BrD " and resid 68   and name HE% )
   (( segid "BrD " and resid 62   and name HG1 ))
      3.600      3.200      1.900 peak  1134 weight  0.10000E+01 volume  0.60159E+02 ppm1      7.900 ppm2      2.143
OR ( 1134)
   (  segid "BrD " and resid 68   and name HE% )
   (( segid "BrD " and resid 73   and name HG  ))
ASSI ( 1164)
   (  segid "BrD " and resid 68   and name HE% )
   (( segid "BrD " and resid 62   and name HG1 ))
      3.200      2.600      2.300 peak  1164 weight  0.10000E+01 volume  0.12306E+03 ppm1      7.896 ppm2      2.374
OR ( 1164)
   (  segid "BrD " and resid 68   and name HE% )
   (( segid "BrD " and resid 73   and name HG  ))
OR ( 1164)
   (  segid "BrD " and resid 107  and name HE% )
   (( segid "BrD " and resid 116  and name HB  ))
ASSI ( 1204)
   (  segid "BrD " and resid 68   and name HE% )
   (( segid "BrD " and resid 68   and name HB2 ))
      2.500      1.600      1.600 peak  1204 weight  0.10000E+01 volume  0.47618E+03 ppm1      7.892 ppm2      3.546
OR ( 1204)
   (  segid "BrD " and resid 68   and name HE% )
   (( segid "BrD " and resid 67   and name HB1 ))
OR ( 1204)
   (  segid "BrD " and resid 107  and name HE% )
   (( segid "BrD " and resid 82   and name HB2 ))
OR ( 1204)
   (( segid "BrD " and resid 34   and name HZ  ))
   (( segid "BrD " and resid 82   and name HB2 ))
ASSI ( 1244)
   (  segid "BrD " and resid 107  and name HE% )
   (( segid "BrD " and resid 79   and name HB2 ))
      2.500      1.600      1.600 peak  1244 weight  0.10000E+01 volume  0.54491E+03 ppm1      7.891 ppm2      2.644
OR ( 1244)
   (  segid "BrD " and resid 68   and name HE% )
   (( segid "BrD " and resid 62   and name HD2 ))
ASSI ( 1254)
   (  segid "BrD " and resid 107  and name HE% )
   (( segid "BrD " and resid 116  and name HG11))
      2.700      1.800      1.800 peak  1254 weight  0.10000E+01 volume  0.30083E+03 ppm1      7.891 ppm2      1.886
OR ( 1254)
   (  segid "BrD " and resid 68   and name HE% )
   (  segid "BrD " and resid 59   and name HE% )
OR ( 1254)
   (  segid "BrD " and resid 107  and name HE% )
   (( segid "BrD " and resid 103  and name HB2 ))
ASSI ( 1274)
   (( segid "BrD " and resid 34   and name HZ  ))
   (( segid "BrD " and resid 98   and name HA  ))
      3.400      2.900      2.100 peak  1274 weight  0.10000E+01 volume  0.84175E+02 ppm1      7.888 ppm2      4.815
OR ( 1274)
   (  segid "BrD " and resid 68   and name HE% )
   (( segid "BrD " and resid 73   and name HA  ))
ASSI ( 1284)
   (  segid "BrD " and resid 107  and name HE% )
   (( segid "BrD " and resid 103  and name HG2 ))
      2.500      1.600      1.600 peak  1284 weight  0.10000E+01 volume  0.45504E+03 ppm1      7.889 ppm2      2.554
OR ( 1284)
   (  segid "BrD " and resid 68   and name HE% )
   (( segid "BrD " and resid 54   and name HB1 ))
ASSI ( 1294)
   (  segid "BrD " and resid 107  and name HE% )
   (( segid "BrD " and resid 116  and name HB  ))
      3.100      2.700      2.200 peak  1294 weight  0.10000E+01 volume  0.10144E+03 ppm1      7.888 ppm2      3.422
OR ( 1294)
   (( segid "BrD " and resid 34   and name HZ  ))
   (( segid "BrD " and resid 101  and name HG11))
ASSI ( 1304)
   (  segid "BrD " and resid 68   and name HE% )
   (  segid "BrD " and resid 58   and name HG2%)
      2.600      1.700      1.700 peak  1304 weight  0.10000E+01 volume  0.38056E+03 ppm1      7.888 ppm2      1.656
OR ( 1304)
   (  segid "BrD " and resid 107  and name HE% )
   (( segid "BrD " and resid 110  and name HG12))
ASSI ( 1444)
   (  segid "BrD " and resid 107  and name HD% )
   (( segid "BrD " and resid 104  and name HA  ))
      2.900      2.100      2.100 peak  1444 weight  0.10000E+01 volume  0.19434E+03 ppm1      7.811 ppm2      4.684
OR ( 1444)
   (  segid "BrD " and resid 105  and name HD% )
   (( segid "BrD " and resid 104  and name HA  ))
OR ( 1444)
   (  segid "BrD " and resid 107  and name HD% )
   (( segid "BrD " and resid 118  and name HA  ))
OR ( 1444)
   (  segid "BrD " and resid 105  and name HD% )
   (( segid "BrD " and resid 109  and name HA  ))
ASSI ( 1504)
   (  segid "BrD " and resid 105  and name HD% )
   (( segid "BrD " and resid 105  and name HA  ))
      2.400      1.400      1.400 peak  1504 weight  0.10000E+01 volume  0.65395E+03 ppm1      7.798 ppm2      4.926
OR ( 1504)
   (  segid "BrD " and resid 68   and name HD% )
   (( segid "BrD " and resid 59   and name HA  ))
ASSI ( 1514)
   (  segid "BrD " and resid 107  and name HD% )
   (( segid "BrD " and resid 106  and name HA  ))
      2.800      2.000      2.000 peak  1514 weight  0.10000E+01 volume  0.27794E+03 ppm1      7.798 ppm2      4.572
OR ( 1514)
   (  segid "BrD " and resid 105  and name HD% )
   (( segid "BrD " and resid 106  and name HA  ))
OR ( 1514)
   (  segid "BrD " and resid 105  and name HD% )
   (( segid "BrD " and resid 108  and name HB1 ))
ASSI ( 1534)
   (  segid "BrD " and resid 105  and name HD% )
   (( segid "BrD " and resid 105  and name HB2 ))
      2.200      1.200      1.200 peak  1534 weight  0.10000E+01 volume  0.11824E+04 ppm1      7.799 ppm2      3.674
OR ( 1534)
   (  segid "BrD " and resid 107  and name HD% )
   (( segid "BrD " and resid 107  and name HB1 ))
OR ( 1534)
   (  segid "BrD " and resid 68   and name HD% )
   (( segid "BrD " and resid 68   and name HB1 ))
ASSI ( 1554)
   (  segid "BrD " and resid 34   and name HE% )
   (( segid "BrD " and resid 102  and name HB2 ))
      2.500      2.500      2.000 peak  1554 weight  0.10000E+01 volume  0.46212E+03 ppm1      7.799 ppm2      1.819
OR ( 1554)
   (  segid "BrD " and resid 68   and name HD% )
   (  segid "BrD " and resid 59   and name HE% )
ASSI ( 1574)
   (  segid "BrD " and resid 105  and name HD% )
   (( segid "BrD " and resid 102  and name HA  ))
      2.800      2.000      2.000 peak  1574 weight  0.10000E+01 volume  0.27340E+03 ppm1      7.797 ppm2      4.278
OR ( 1574)
   (  segid "BrD " and resid 105  and name HD% )
   (( segid "BrD " and resid 101  and name HA  ))
OR ( 1574)
   (  segid "BrD " and resid 34   and name HE% )
   (( segid "BrD " and resid 102  and name HA  ))
ASSI ( 1614)
   (  segid "BrD " and resid 68   and name HD% )
   (( segid "BrD " and resid 74   and name HB2 ))
      2.900      2.100      2.100 peak  1614 weight  0.10000E+01 volume  0.20510E+03 ppm1      7.790 ppm2      3.010
OR ( 1614)
   (  segid "BrD " and resid 105  and name HD% )
   (( segid "BrD " and resid 109  and name HE2 ))
ASSI ( 1624)
   (  segid "BrD " and resid 34   and name HE% )
   (( segid "BrD " and resid 33   and name HD1 ))
      2.800      2.000      2.000 peak  1624 weight  0.10000E+01 volume  0.23703E+03 ppm1      7.786 ppm2      2.796
OR ( 1624)
   (( segid "BrD " and resid 32   and name HZ3 ))
   (( segid "BrD " and resid 33   and name HD1 ))
OR ( 1624)
   (  segid "BrD " and resid 107  and name HD% )
   (( segid "BrD " and resid 79   and name HB1 ))
OR ( 1624)
   (( segid "BrD " and resid 32   and name HH2 ))
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   (( segid "BrD " and resid 33   and name HD1 ))
ASSI { 1654}
   ( segid "BrD " and resid 34   and name HE% )
   (( segid "BrD " and resid 85   and name HB1 ))
     2.400      1.700      1.700 peak  1654 weight  0.10000E+01 volume  0.36960E+03 ppm1       7.784 ppm2       3.920
OR { 1654}
   ( segid "BrD " and resid 107  and name HD% )
   (( segid "BrD " and resid 106  and name HB1 ))
ASSI { 1664}
   ( segid "BrD " and resid 34   and name HE% )
   ( segid "BrD " and resid 99   and name HB% )
     2.400      1.400      1.400 peak  1664 weight  0.10000E+01 volume  0.66064E+03 ppm1       7.786 ppm2       2.211
OR { 1664}
   ( segid "BrD " and resid 34   and name HE% )
   (( segid "BrD " and resid 33   and name HD2 ))
ASSI { 1674}
   (( segid "BrD " and resid 32   and name HH2 ))
   (( segid "BrD " and resid 33   and name HG1 ))
     3.300      2.700      2.200 peak  1674 weight  0.10000E+01 volume  0.96896E+02 ppm1       7.786 ppm2       0.876
OR { 1674}
   (( segid "BrD " and resid 32   and name HZ3 ))
   (( segid "BrD " and resid 33   and name HG1 ))
OR { 1674}
   ( segid "BrD " and resid 34   and name HE% )
   (( segid "BrD " and resid 33   and name HG1 ))
ASSI { 1684}
   ( segid "BrD " and resid 34   and name HE% )
   (( segid "BrD " and resid 98   and name HA  ))
     3.400      2.900      2.100 peak  1684 weight  0.10000E+01 volume  0.73775E+02 ppm1       7.783 ppm2       4.815
OR { 1684}
   (( segid "BrD " and resid 32   and name HH2 ))
   (( segid "BrD " and resid 94   and name HA  ))
OR { 1684}
   ( segid "BrD " and resid 68   and name HD% )
   (( segid "BrD " and resid 73   and name HA  ))
OR { 1684}
   ( segid "BrD " and resid 107  and name HD% )
   (( segid "BrD " and resid 108  and name HA  ))
OR { 1684}
   ( segid "BrD " and resid 68   and name HD% )
   (( segid "BrD " and resid 60   and name HA  ))
OR { 1684}
   (( segid "BrD " and resid 32   and name HH2 ))
   (( segid "BrD " and resid 98   and name HA  ))
OR { 1684}
   ( segid "BrD " and resid 34   and name HE% )
   (( segid "BrD " and resid 86   and name HA  ))
OR { 1684}
   ( segid "BrD " and resid 107  and name HD% )
   (( segid "BrD " and resid 116  and name HA  ))
OR { 1684}
   ( segid "BrD " and resid 105  and name HD% )
   (( segid "BrD " and resid 108  and name HA  ))
OR { 1684}
   (( segid "BrD " and resid 32   and name HZ3 ))
   (( segid "BrD " and resid 94   and name HA  ))
ASSI { 1704}
   ( segid "BrD " and resid 68   and name HD% )
   (( segid "BrD " and resid 62   and name HD1 ))
     2.700      1.800      1.800 peak  1704 weight  0.10000E+01 volume  0.31213E+03 ppm1       7.787 ppm2       3.153
OR { 1704}
   ( segid "BrD " and resid 105  and name HD% )
   (( segid "BrD " and resid 109  and name HE1 ))
ASSI { 1714}
   ( segid "BrD " and resid 68   and name HD% )
   (( segid "BrD " and resid 62   and name HB1 ))
     2.300      1.300      1.300 peak  1714 weight  0.10000E+01 volume  0.79418E+03 ppm1       7.779 ppm2       2.602
OR { 1714}
   ( segid "BrD " and resid 107  and name HD% )
   (( segid "BrD " and resid 103  and name HG1 ))
OR { 1714}
   ( segid "BrD " and resid 68   and name HD% )
   (( segid "BrD " and resid 62   and name HD2 ))
ASSI { 1734}
   ( segid "BrD " and resid 68   and name HD% )
   (( segid "BrD " and resid 62   and name HG1 ))
     2.900      2.100      2.100 peak  1734 weight  0.10000E+01 volume  0.18466E+03 ppm1       7.781 ppm2       2.324
OR { 1734}
   ( segid "BrD " and resid 34   and name HE% )
   ( segid "BrD " and resid 31   and name HB% )
OR { 1734}
   ( segid "BrD " and resid 107  and name HD% )
   (( segid "BrD " and resid 110  and name HB  ))
OR { 1734}
   ( segid "BrD " and resid 68   and name HD% )
   (( segid "BrD " and resid 73   and name HG  ))
ASSI { 1744}
   ( segid "BrD " and resid 107  and name HD% )
   (( segid "BrD " and resid 110  and name HG12 ))
     2.300      1.300      1.300 peak  1744 weight  0.10000E+01 volume  0.92480E+03 ppm1       7.761 ppm2       1.641
OR { 1744}
   ( segid "BrD " and resid 34   and name HE% )
   ( segid "BrD " and resid 25   and name HG2% )
ASSI { 1784}
   ( segid "BrD " and resid 68   and name HD% )
   (( segid "BrD " and resid 62   and name HG1 ))
     2.800      2.000      2.000 peak  1784 weight  0.10000E+01 volume  0.26728E+03 ppm1       7.781 ppm2       2.374
OR { 1784}
   ( segid "BrD " and resid 107  and name HD% )
   (( segid "BrD " and resid 110  and name HB  ))
OR { 1784}
   ( segid "BrD " and resid 68   and name HD% )
   (( segid "BrD " and resid 73   and name HG  ))
ASSI { 1804}
   ( segid "BrD " and resid 68   and name HD% )
   (( segid "BrD " and resid 62   and name HG2 ))
     2.700      1.800      1.800 peak  1804 weight  0.10000E+01 volume  0.30580E+03 ppm1       7.781 ppm2       1.503
OR { 1804}
   ( segid "BrD " and resid 68   and name HD% )
   ( segid "BrD " and resid 73   and name HD2% )
ASSI { 1884}
   ( segid "BrD " and resid 96   and name HD% )
   (( segid "BrD " and resid 92   and name HB1 ))
     2.900      2.100      2.100 peak  1884 weight  0.10000E+01 volume  0.22072E+03 ppm1       7.726 ppm2       2.666
OR { 1884}
   ( segid "BrD " and resid 34   and name HD% )
   (( segid "BrD " and resid 56   and name HB1 ))
ASSI { 1924}
   ( segid "BrD " and resid 96   and name HD% )
   ( segid "BrD " and resid 99   and name HB% )
     2.500      1.600      1.600 peak  1924 weight  0.10000E+01 volume  0.65506E+03 ppm1       7.721 ppm2       3.211
OR { 1924}
   ( segid "BrD " and resid 34   and name HD% )
   (( segid "BrD " and resid 33   and name HD2 ))
ASSI { 1964}
   ( segid "BrD " and resid 96   and name HD% )
   (( segid "BrD " and resid 92   and name HG1 ))
     2.800      2.000      2.000 peak  1964 weight  0.10000E+01 volume  0.22599E+03 ppm1       7.714 ppm2       2.796
OR { 1964}
   ( segid "BrD " and resid 34   and name HD% )
   (( segid "BrD " and resid 33   and name HD1 ))
OR { 1964}
   ( segid "BrD " and resid 34   and name HD% )
   ( segid "BrD " and resid 35   and name HE% )
ASSI { 1974}
   ( segid "BrD " and resid 96   and name HD% )
   (( segid "BrD " and resid 86   and name HB1 ))
     2.300      2.300      2.200 peak  1974 weight  0.10000E+01 volume  0.79213E+03 ppm1       7.717 ppm2       2.321
OR { 1974}
   ( segid "BrD " and resid 34   and name HD% )
   ( segid "BrD " and resid 31   and name HB% )
ASSI { 1994}
   ( segid "BrD " and resid 34   and name HD% )
   ( segid "BrD " and resid 81   and name HG2% )
     2.400      1.400      1.400 peak  1994 weight  0.10000E+01 volume  0.69140E+03 ppm1       7.717 ppm2       0.762
OR { 1994}
   ( segid "BrD " and resid 96   and name HD% )
   (( segid "BrD " and resid 86   and name HG2 ))
ASSI { 2054}
   ( segid "BrD " and resid 34   and name HD% )
   (( segid "BrD " and resid 61   and name HB  ))
     2.900      2.100      2.100 peak  2054 weight  0.10000E+01 volume  0.18901E+03 ppm1       7.709 ppm2       2.033
OR { 2054}
   ( segid "BrD " and resid 34   and name HD% )
   (( segid "BrD " and resid 56   and name HB2 ))
ASSI { 2064}
   ( segid "BrD " and resid 34   and name HD% )
   (( segid "BrD " and resid 33   and name HB1 ))
     2.800      2.000      2.000 peak  2064 weight  0.10000E+01 volume  0.24003E+03 ppm1       7.714 ppm2       1.086
OR { 2064}
   ( segid "BrD " and resid 34   and name HD% )
   ( segid "BrD " and resid 61   and name HG1% )
ASSI { 2134}
   ( segid "BrD " and resid 15   and name HD% )
   (( segid "BrD " and resid 19   and name HE1 ))
     4.000      4.000      1.500 peak  2134 weight  0.10000E+01 volume  0.29314E+02 ppm1       7.692 ppm2       3.512
OR { 2134}
   ( segid "BrD " and resid 96   and name HD% )
   (( segid "BrD " and resid 89   and name HB2 ))
ASSI { 2274}
   ( segid "BrD " and resid 106  and name HE% )
   ( segid "BrD " and resid 59   and name HE% )
     3.400      2.900      2.100 peak  2274 weight  0.10000E+01 volume  0.79128E+02 ppm1       7.640 ppm2       1.820
OR { 2274}
   ( segid "BrD " and resid 106  and name HE% )
   ( segid "BrD " and resid 25   and name HG1% )
ASSI { 2294}
   ( segid "BrD " and resid 106  and name HE% )
   ( segid "BrD " and resid 21   and name HG2% )
     2.600      1.700      1.700 peak  2294 weight  0.10000E+01 volume  0.41702E+03 ppm1       7.643 ppm2       1.593
OR { 2294}
   ( segid "BrD " and resid 106  and name HE% )
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  (( segid "BrD " and resid 116  and name HG12))
ASSI ( 2314)
  (  segid "BrD " and resid 106  and name HE% )
  (( segid "BrD " and resid 106  and name HB2 ))
     4.000     4.000     1.500 peak  2314 weight  0.10000E+01 volume  0.29199E+02 ppm1      7.633 ppm2      3.691
OR ( 2314)
  (  segid "BrD " and resid 95   and name HE% )
  (( segid "BrD " and resid 89   and name HB1 ))
OR ( 2314)
  (  segid "BrD " and resid 88   and name HD% )
  (( segid "BrD " and resid 89   and name HB1 ))
OR ( 2314)
  (  segid "BrD " and resid 106  and name HE% )
  (( segid "BrD " and resid 107  and name HB1 ))
ASSI ( 2324)
  (  segid "BrD " and resid 106  and name HE% )
  (  segid "BrD " and resid 21   and name HG2%)
     2.600     1.700     1.700 peak  2324 weight  0.10000E+01 volume  0.43383E+03 ppm1      7.616 ppm2      1.576
OR ( 2324)
  (  segid "BrD " and resid 88   and name HD% )
  (  segid "BrD " and resid 49   and name HG2%)
OR ( 2324)
  (  segid "BrD " and resid 106  and name HE% )
  (( segid "BrD " and resid 116  and name HG12))
ASSI ( 2334)
  (  segid "BrD " and resid 95   and name HE% )
  (( segid "BrD " and resid 33   and name HB1 ))
     2.900     2.100     2.100 peak  2334 weight  0.10000E+01 volume  0.19423E+03 ppm1      7.623 ppm2      1.095
OR ( 2334)
  (  segid "BrD " and resid 106  and name HE% )
  (  segid "BrD " and resid 18   and name HD1%)
ASSI ( 2344)
  (  segid "BrD " and resid 95   and name HE% )
  (( segid "BrD " and resid 32   and name HZ2 ))
     3.100     2.700     2.200 peak  2344 weight  0.10000E+01 volume  0.91993E+02 ppm1      7.615 ppm2      8.004
OR ( 2344)
  (  segid "BrD " and resid 106  and name HE% )
  (( segid "BrD " and resid 107  and name HZ  ))
ASSI ( 2354)
  (  segid "BrD " and resid 95   and name HE% )
  (( segid "BrD " and resid 95   and name HA  ))
     3.000     2.200     2.200 peak  2354 weight  0.10000E+01 volume  0.18109E+03 ppm1      7.619 ppm2      4.448
OR ( 2354)
  (  segid "BrD " and resid 96   and name HE% )
  (( segid "BrD " and resid 96   and name HA  ))
OR ( 2354)
  (  segid "BrD " and resid 106  and name HE% )
  (( segid "BrD " and resid 107  and name HA  ))
OR ( 2354)
  (  segid "BrD " and resid 106  and name HE% )
  (( segid "BrD " and resid 79   and name HA  ))
ASSI ( 2364)
  (  segid "BrD " and resid 95   and name HE% )
  (( segid "BrD " and resid 33   and name HA  ))
     3.200     2.600     2.300 peak  2364 weight  0.10000E+01 volume  0.11374E+03 ppm1      7.617 ppm2      4.366
OR ( 2364)
  (  segid "BrD " and resid 106  and name HE% )
  (( segid "BrD " and resid 21   and name HA  ))
ASSI ( 2374)
  (  segid "BrD " and resid 88   and name HD% )
  (( segid "BrD " and resid 87   and name HB1 ))
     3.000     2.200     2.200 peak  2374 weight  0.10000E+01 volume  0.17346E+03 ppm1      7.619 ppm2      2.771
OR ( 2374)
  (  segid "BrD " and resid 106  and name HE% )
  (( segid "BrD " and resid 79   and name HB1 ))
OR ( 2374)
  (  segid "BrD " and resid 95   and name HE% )
  (( segid "BrD " and resid 33   and name HD1 ))
OR ( 2374)
  (  segid "BrD " and resid 88   and name HD% )
  (( segid "BrD " and resid 87   and name HG2 ))
ASSI ( 2404)
  (  segid "BrD " and resid 106  and name HE% )
  (  segid "BrD " and resid 75   and name HE% )
     2.800     2.000     2.000 peak  2404 weight  0.10000E+01 volume  0.24430E+03 ppm1      7.615 ppm2      2.618
OR ( 2404)
  (  segid "BrD " and resid 88   and name HD% )
  (( segid "BrD " and resid 49   and name HB  ))
ASSI ( 2424)
  (  segid "BrD " and resid 88   and name HD% )
  (  segid "BrD " and resid 49   and name HG1%)
     2.600     1.700     1.700 peak  2424 weight  0.10000E+01 volume  0.35330E+03 ppm1      7.616 ppm2      1.658
OR ( 2424)
  (  segid "BrD " and resid 106  and name HE% )
  (( segid "BrD " and resid 21   and name HG12))
ASSI ( 2454)
  (  segid "BrD " and resid 106  and name HE% )
  (( segid "BrD " and resid 17   and name HB  ))
     2.500     1.600     1.600 peak  2454 weight  0.10000E+01 volume  0.48101E+03 ppm1      7.611 ppm2      4.815
OR ( 2454)
  (  segid "BrD " and resid 96   and name HE% )
  (( segid "BrD " and resid 86   and name HA  ))
OR ( 2454)
  (  segid "BrD " and resid 96   and name HE% )
  (( segid "BrD " and resid 97   and name HA  ))
OR ( 2454)
  (  segid "BrD " and resid 88   and name HD% )
  (( segid "BrD " and resid 87   and name HA  ))
OR ( 2454)
  (  segid "BrD " and resid 96   and name HE% )
  (( segid "BrD " and resid 92   and name HA  ))
OR ( 2454)
  (  segid "BrD " and resid 95   and name HE% )
  (( segid "BrD " and resid 94   and name HA  ))
ASSI ( 2524)
  (  segid "BrD " and resid 106  and name HE% )
  (( segid "BrD " and resid 116  and name HG11))
     3.000     2.200     2.200 peak  2524 weight  0.10000E+01 volume  0.18273E+03 ppm1      7.611 ppm2      1.925
OR ( 2524)
  (  segid "BrD " and resid 96   and name HE% )
  (( segid "BrD " and resid 86   and name HG1 ))
OR ( 2524)
  (  segid "BrD " and resid 96   and name HE% )
  (( segid "BrD " and resid 86   and name HD1 ))
ASSI ( 2544)
  (  segid "BrD " and resid 106  and name HD% )
  (( segid "BrD " and resid 107  and name HA  ))
     3.100     2.400     2.400 peak  2544 weight  0.10000E+01 volume  0.12798E+03 ppm1      7.538 ppm2      4.390
OR ( 2544)
  (  segid "BrD " and resid 106  and name HD% )
  (( segid "BrD " and resid 79   and name HA  ))
OR ( 2544)
  (  segid "BrD " and resid 74   and name HE% )
  (( segid "BrD " and resid 74   and name HA  ))
ASSI ( 2604)
  (  segid "BrD " and resid 74   and name HE% )
  (( segid "BrD " and resid 59   and name HB1 ))
     2.500     1.600     1.600 peak  2604 weight  0.10000E+01 volume  0.55016E+03 ppm1      7.534 ppm2      2.695
OR ( 2604)
  (  segid "BrD " and resid 74   and name HE% )
  (( segid "BrD " and resid 22   and name HB1 ))
ASSI ( 2624)
  (  segid "BrD " and resid 106  and name HD% )
  (( segid "BrD " and resid 109  and name HB2 ))
     3.000     2.200     2.200 peak  2624 weight  0.10000E+01 volume  0.15519E+03 ppm1      7.534 ppm2      2.166
OR ( 2624)
  (  segid "BrD " and resid 74   and name HE% )
  (( segid "BrD " and resid 18   and name HB1 ))
ASSI ( 2644)
  (  segid "BrD " and resid 74   and name HE% )
  (( segid "BrD " and resid 63   and name HB2 ))
     2.300     1.300     1.300 peak  2644 weight  0.10000E+01 volume  0.82012E+03 ppm1      7.531 ppm2      2.521
OR ( 2644)
  (  segid "BrD " and resid 106  and name HD% )
  (( segid "BrD " and resid 21   and name HB  ))
ASSI ( 2664)
  (  segid "BrD " and resid 106  and name HD% )
  (  segid "BrD " and resid 102  and name HD2%)
     2.800     2.000     2.000 peak  2664 weight  0.10000E+01 volume  0.24374E+03 ppm1      7.530 ppm2      1.331
OR ( 2664)
  (  segid "BrD " and resid 74   and name HE% )
  (( segid "BrD " and resid 74   and name HB1 ))
ASSI ( 2784)
  (  segid "BrD " and resid 74   and name HE% )
  (( segid "BrD " and resid 68   and name HB2 ))
     2.900     2.100     2.100 peak  2784 weight  0.10000E+01 volume  0.21978E+03 ppm1      7.530 ppm2      3.559
OR ( 2784)
  (  segid "BrD " and resid 74   and name HE% )
  (( segid "BrD " and resid 74   and name HB1 ))
OR ( 2784)
  (  segid "BrD " and resid 95   and name HD% )
  (( segid "BrD " and resid 88   and name HB1 ))
ASSI ( 2804)
  (  segid "BrD " and resid 95   and name HD% )
  (( segid "BrD " and resid 32   and name HH2 ))
     2.800     2.000     2.000 peak  2804 weight  0.10000E+01 volume  0.23332E+03 ppm1      7.520 ppm2      7.793
OR ( 2804)
  (  segid "BrD " and resid 106  and name HD% )
  (  segid "BrD " and resid 107  and name HD% )
ASSI ( 2814)
  (  segid "BrD " and resid 106  and name HD% )
  (( segid "BrD " and resid 78   and name HB2 ))
     3.000     3.200     2.200 peak  2814 weight  0.10000E+01 volume  0.16253E+03 ppm1      7.520 ppm2      1.080
OR ( 2814)
  (  segid "BrD " and resid 74   and name HE% )
  (  segid "BrD " and resid 18   and name HD1%)
OR ( 2814)
  (  segid "BrD " and resid 95   and name HD% )
  (( segid "BrD " and resid 33   and name HB1 ))
ASSI ( 2914)
  (  segid "BrD " and resid 18   and name HE% )
  (( segid "BrD " and resid 19   and name HE1 ))
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     2.900      2.100      2.100 peak  2914 weight  0.10000E+01 volume  0.20135E+03 ppm1      7.488 ppm2      3.545
OR ( 2914)
   (  segid "BrD " and resid 95    and name HD% )
   (( segid "BrD " and resid 86    and name HB1 ))
ASSI ( 3164)
   (  segid "BrD " and resid 82    and name HD% )
   (( segid "BrD " and resid 103   and name HB1 ))
     2.700      1.800      1.800 peak  3164 weight  0.10000E+01 volume  0.29307E+03 ppm1      7.270 ppm2      2.309
OR ( 3164)
   (  segid "BrD " and resid 47    and name HE% )
   (( segid "BrD " and resid 37    and name HB2 ))
ASSI ( 3284)
   (  segid "BrD " and resid 82    and name HD% )
   (  segid "BrD " and resid 34    and name HE% )
     2.800      2.000      2.000 peak  3284 weight  0.10000E+01 volume  0.24491E+03 ppm1      7.263 ppm2      7.800
OR ( 3284)
   (  segid "BrD " and resid 82    and name HD% )
   (  segid "BrD " and resid 107   and name HD% )
ASSI ( 3324)
   (  segid "BrD " and resid 82    and name HE% )
   (( segid "BrD " and resid 79    and name HA  ))
     2.900      2.100      2.100 peak  3324 weight  0.10000E+01 volume  0.20070E+03 ppm1      7.074 ppm2      4.440
OR ( 3324)
   (  segid "BrD " and resid 82    and name HE% )
   (( segid "BrD " and resid 107   and name HA  ))
ASSI ( 3394)
   (  segid "BrD " and resid 82    and name HE% )
   (( segid "BrD " and resid 81    and name HB  ))
     2.600      1.700      1.700 peak  3394 weight  0.10000E+01 volume  0.37624E+03 ppm1      7.069 ppm2      2.012
OR ( 3394)
   (  segid "BrD " and resid 82    and name HE% )
   (( segid "BrD " and resid 102   and name HB1 ))
ASSI ( 3414)
   (  segid "BrD " and resid 82    and name HE% )
   (  segid "BrD " and resid 25    and name HG2%)
     3.400      2.900      2.100 peak  3414 weight  0.10000E+01 volume  0.73603E+02 ppm1      7.067 ppm2      1.641
OR ( 3414)
   (  segid "BrD " and resid 82    and name HE% )
   (( segid "BrD " and resid 110   and name HG12))
ASSI ( 3474)
   (( segid "BrD " and resid 82    and name HZ  ))
   (( segid "BrD " and resid 102   and name HG  ))
     2.800      2.000      2.000 peak  3474 weight  0.10000E+01 volume  0.23859E+03 ppm1      7.025 ppm2      2.163
OR ( 3474)
   (  segid "BrD " and resid 74    and name HD% )
   (( segid "BrD " and resid 18    and name HB1 ))
ASSI ( 3484)
   (  segid "BrD " and resid 74    and name HD% )
   (  segid "BrD " and resid 78    and name HD1%)
     2.900      2.100      2.100 peak  3484 weight  0.10000E+01 volume  0.18792E+03 ppm1      7.023 ppm2      0.780
OR ( 3484)
   (( segid "BrD " and resid 82    and name HZ  ))
   (  segid "BrD " and resid 78    and name HD1%)
ASSI ( 3494)
   (  segid "BrD " and resid 74    and name HD% )
   (( segid "BrD " and resid 68    and name HB1 ))
     2.900      2.100      2.100 peak  3494 weight  0.10000E+01 volume  0.19853E+03 ppm1      7.022 ppm2      3.708
OR ( 3494)
   (( segid "BrD " and resid 82    and name HZ  ))
   (( segid "BrD " and resid 106   and name HB2 ))
ASSI ( 3504)
   (( segid "BrD " and resid 82    and name HZ  ))
   (( segid "BrD " and resid 81    and name HB  ))
     3.100      2.400      2.400 peak  3504 weight  0.10000E+01 volume  0.12383E+03 ppm1      7.023 ppm2      2.034
OR ( 3504)
   (  segid "BrD " and resid 74    and name HD% )
   (( segid "BrD " and resid 14    and name HG  ))
ASSI ( 3544)
   (  segid "BrD " and resid 74    and name HD% )
   (( segid "BrD " and resid 18    and name HG  ))
     3.400      2.900      2.100 peak  3544 weight  0.10000E+01 volume  0.82384E+02 ppm1      7.005 ppm2      2.307
OR ( 3544)
   (( segid "BrD " and resid 82    and name HZ  ))
   (( segid "BrD " and resid 103   and name HB1 ))
OR ( 3544)
   (  segid "BrD " and resid 74    and name HD% )
   (( segid "BrD " and resid 21    and name HG11))
OR ( 3544)
   (  segid "BrD " and resid 74    and name HD% )
   (( segid "BrD " and resid 62    and name HG1 ))
OR ( 3544)
   (  segid "BrD " and resid 74    and name HD% )
   (( segid "BrD " and resid 73    and name HG  ))
OR ( 3544)
   (( segid "BrD " and resid 82    and name HZ  ))
   (( segid "BrD " and resid 21    and name HG11))
ASSI ( 3554)
   (  segid "BrD " and resid 74    and name HD% )
   (  segid "BrD " and resid 63    and name HD1%)
     2.500      1.600      1.600 peak  3554 weight  0.10000E+01 volume  0.51806E+03 ppm1      7.009 ppm2      1.641
OR ( 3554)
   (  segid "BrD " and resid 74    and name HD% )
   (  segid "BrD " and resid 22    and name HD1%)
ASSI ( 3564)
   (  segid "BrD " and resid 74    and name HD% )
   (  segid "BrD " and resid 68    and name HE% )
     3.100      2.400      2.400 peak  3564 weight  0.10000E+01 volume  0.13987E+03 ppm1      7.005 ppm2      7.689
OR ( 3564)
   (( segid "BrD " and resid 82    and name HZ  ))
   (  segid "BrD " and resid 107   and name HE% )
ASSI ( 3584)
   (  segid "BrD " and resid 74    and name HD% )
   (  segid "BrD " and resid 106   and name HE% )
     3.000      2.200      2.200 peak  3584 weight  0.10000E+01 volume  0.17632E+03 ppm1      7.005 ppm2      7.647
OR ( 3584)
   (( segid "BrD " and resid 82    and name HZ  ))
   (  segid "BrD " and resid 106   and name HE% )
ASSI ( 3604)
   (  segid "BrD " and resid 74    and name HD% )
   (( segid "BrD " and resid 71    and name HA  ))
     3.300      2.700      2.200 peak  3604 weight  0.10000E+01 volume  0.95504E+02 ppm1      7.005 ppm2      4.636
OR ( 3604)
   (  segid "BrD " and resid 74    and name HD% )
   (( segid "BrD " and resid 15    and name HA  ))
OR ( 3604)
   (  segid "BrD " and resid 74    and name HD% )
   (( segid "BrD " and resid 76    and name HA  ))
OR ( 3604)
   (  segid "BrD " and resid 74    and name HD% )
   (( segid "BrD " and resid 56    and name HA  ))
OR ( 3604)
   (  segid "BrD " and resid 74    and name HD% )
   (( segid "BrD " and resid 72    and name HA  ))
OR ( 3604)
   (  segid "BrD " and resid 74    and name HD% )
   (( segid "BrD " and resid 14    and name HA  ))
OR ( 3604)
   (  segid "BrD " and resid 74    and name HD% )
   (( segid "BrD " and resid 67    and name HA  ))
OR ( 3604)
   (  segid "BrD " and resid 74    and name HD% )
   (( segid "BrD " and resid 60    and name HB2 ))
OR ( 3604)
   (( segid "BrD " and resid 82    and name HZ  ))
   (( segid "BrD " and resid 106   and name HA  ))
ASSI ( 3634)
   (  segid "BrD " and resid 74    and name HD% )
   (( segid "BrD " and resid 75    and name HG2 ))
     3.100      2.400      2.400 peak  3634 weight  0.10000E+01 volume  0.12756E+03 ppm1      7.004 ppm2      3.221
OR ( 3634)
   (  segid "BrD " and resid 74    and name HD% )
   (( segid "BrD " and resid 59    and name HG1 ))
OR ( 3634)
   (  segid "BrD " and resid 74    and name HD% )
   (( segid "BrD " and resid 59    and name HG2 ))
ASSI ( 3664)
   (  segid "BrD " and resid 74    and name HD% )
   (( segid "BrD " and resid 63    and name HB2 ))
     3.600      3.200      1.900 peak  3664 weight  0.10000E+01 volume  0.57581E+02 ppm1      7.005 ppm2      2.520
OR ( 3664)
   (( segid "BrD " and resid 82    and name HZ  ))
   (( segid "BrD " and resid 21    and name HB  ))
ASSI ( 3674)
   (( segid "BrD " and resid 82    and name HZ  ))
   (( segid "BrD " and resid 21    and name HB  ))
     3.700      3.400      1.800 peak  3674 weight  0.10000E+01 volume  0.46728E+02 ppm1      7.004 ppm2      2.494
OR ( 3674)
   (  segid "BrD " and resid 74    and name HD% )
   (( segid "BrD " and resid 59    and name HB2 ))
OR ( 3674)
   (  segid "BrD " and resid 74    and name HD% )
   (( segid "BrD " and resid 73    and name HB2 ))
ASSI ( 3694)
   (  segid "BrD " and resid 74    and name HD% )
   (  segid "BrD " and resid 63    and name HD2%)
     3.800      3.100      2.000 peak  3694 weight  0.10000E+01 volume  0.62447E+02 ppm1      7.005 ppm2      1.496
OR ( 3694)
   (  segid "BrD " and resid 74    and name HD% )
   (  segid "BrD " and resid 73    and name HD2%)
ASSI ( 3854)
   (  segid "BrD " and resid 46    and name HE% )
   (( segid "BrD " and resid 50    and name HG12))
     2.700      1.800      1.800 peak  3854 weight  0.10000E+01 volume  0.29261E+03 ppm1      6.687 ppm2      0.795
OR ( 3854)
   (  segid "BrD " and resid 46    and name HE% )
   (  segid "BrD " and resid 38    and name HG2%)
ASSI ( 3954)
   (  segid "BrD " and resid 46    and name HD% )
   (( segid "BrD " and resid 50    and name HG12))
     3.200      2.600      2.300 peak  3954 weight  0.10000E+01 volume  0.11437E+03 ppm1      5.740 ppm2      0.796
OR ( 3954)
   (  segid "BrD " and resid 46    and name HD% )
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   (  segid "BrD " and resid 38   and name HG2%)
ASSI ( 4144)
   (  segid "BrD " and resid 74   and name HD% )
   (( segid "BrD " and resid 78   and name HG  ))
      3.400     2.900     2.100 peak  4144 weight  0.10000E+01 volume  0.77150E+02 ppm1      7.005 ppm2      1.249
OR ( 4144)
   (( segid "BrD " and resid 82   and name HZ  ))
   (( segid "BrD " and resid 78   and name HG  ))
ASSI ( 4154)
   (  segid "BrD " and resid 74   and name HE% )
   (  segid "BrD " and resid 22   and name HD1%)
      2.400     1.400     1.400 peak  4154 weight  0.10000E+01 volume  0.70341E+03 ppm1      7.534 ppm2      1.676
OR ( 4154)
   (  segid "BrD " and resid 106  and name HD% )
   (( segid "BrD " and resid 21   and name HG12))
ASSI ( 4174)
   (  segid "BrD " and resid 96   and name HD% )
   (( segid "BrD " and resid 100  and name HA  ))
      3.100     2.400     2.400 peak  4174 weight  0.10000E+01 volume  0.13533E+03 ppm1      7.689 ppm2      4.927
OR ( 4174)
   (  segid "BrD " and resid 34   and name HD% )
   (( segid "BrD " and resid 35   and name HA  ))
OR ( 4174)
   (  segid "BrD " and resid 15   and name HD% )
   (( segid "BrD " and resid 64   and name HA  ))
OR ( 4174)
   (  segid "BrD " and resid 15   and name HD% )
   (( segid "BrD " and resid 11   and name HA  ))
OR ( 4174)
   (  segid "BrD " and resid 34   and name HD% )
   (( segid "BrD " and resid 32   and name HA  ))
ASSI ( 4224)
   (  segid "BrD " and resid 68   and name HD% )
   (( segid "BrD " and resid 50   and name HG12))
      3.100     2.400     2.400 peak  4224 weight  0.10000E+01 volume  0.12837E+03 ppm1      7.615 ppm2      0.845
OR ( 4224)
   (  segid "BrD " and resid 95   and name HE% )
   (( segid "BrD " and resid 33   and name HG1 ))
ASSI ( 4234)
   (  segid "BrD " and resid 96   and name HE% )
   (  segid "BrD " and resid 99   and name HB% )
      3.300     2.700     2.200 peak  4234 weight  0.10000E+01 volume  0.94963E+02 ppm1      7.611 ppm2      2.178
OR ( 4234)
   (  segid "BrD " and resid 106  and name HE% )
   (( segid "BrD " and resid 18   and name HB1 ))
OR ( 4234)
   (  segid "BrD " and resid 106  and name HE% )
   (( segid "BrD " and resid 109  and name HB2 ))
OR ( 4234)
   (  segid "BrD " and resid 106  and name HE% )
   (( segid "BrD " and resid 115  and name HB1 ))
OR ( 4234)
   (  segid "BrD " and resid 106  and name HE% )
   (( segid "BrD " and resid 115  and name HG  ))
ASSI ( 4244)
   (  segid "BrD " and resid 106  and name HE% )
   (  segid "BrD " and resid 78   and name HD1%)
      3.100     2.400     2.400 peak  4244 weight  0.10000E+01 volume  0.14012E+03 ppm1      7.616 ppm2      0.763
OR ( 4244)
   (  segid "BrD " and resid 96   and name HE% )
   (( segid "BrD " and resid 86   and name HG2 ))
ASSI ( 4284)
   (  segid "BrD " and resid 74   and name HE% )
   (( segid "BrD " and resid 74   and name HB2 ))
      3.000     2.200     2.200 peak  4284 weight  0.10000E+01 volume  0.18031E+03 ppm1      7.534 ppm2      3.010
OR ( 4284)
   (  segid "BrD " and resid 106  and name HD% )
   (( segid "BrD " and resid 109  and name HE2 ))
ASSI ( 4344)
   (( segid "BrD " and resid 34   and name HZ  ))
   (( segid "BrD " and resid 28   and name HD2 ))
      3.100     2.400     2.400 peak  4344 weight  0.10000E+01 volume  0.12962E+03 ppm1      7.904 ppm2      5.555
OR ( 4344)
   (  segid "BrD " and resid 68   and name HE% )
   (( segid "BrD " and resid 54   and name HA  ))
ASSI ( 4354)
   (  segid "BrD " and resid 106  and name HD% )
   (( segid "BrD " and resid 78   and name HB2 ))
      2.900     2.100     2.100 peak  4354 weight  0.10000E+01 volume  0.19182E+03 ppm1      7.539 ppm2      1.069
OR ( 4354)
   (  segid "BrD " and resid 74   and name HE% )
   (  segid "BrD " and resid 18   and name HD1%)
```

Table 4

Hydrogen Bonding Restraints

```
!Helix Z
assign (residue 19 and name HN  ) (residue 15  and name O )     1.80  0.0  0.40
assign (residue 19 and name N   ) (residue 15  and name O )     2.80  0.30 0.40

assign (residue 22 and name HN  ) (residue 18  and name O )     1.80  0.0  0.40
assign (residue 22 and name N   ) (residue 18  and name O )     2.80  0.30 0.40

assign (residue 23 and name HN  ) (residue 19  and name O )     1.80  0.0  0.40
assign (residue 23 and name N   ) (residue 19  and name O )     2.80  0.30 0.40

assign (residue 24 and name HN  ) (residue 20  and name O )     1.80  0.0  0.40
assign (residue 24 and name N   ) (residue 20  and name O )     2.80  0.30 0.40

assign (residue 25 and name HN  ) (residue 21  and name O )     1.80  0.0  0.40
assign (residue 25 and name N   ) (residue 21  and name O )     2.80  0.30 0.40


!Helix B
assign (residue 75 and name HN  ) (residue 71  and name O )     1.80  0.0  0.40
assign (residue 75 and name N   ) (residue 71  and name O )     2.80  0.30 0.40

!assign (residue 77 and name HN  ) (residue 73  and name O )     1.80  0.0  0.40
!assign (residue 77 and name N   ) (residue 73  and name O )     2.80  0.30 0.40

assign (residue 78 and name HN  ) (residue 74  and name O )     1.80  0.0  0.40
assign (residue 78 and name N   ) (residue 74  and name O )     2.80  0.30 0.40

assign (residue 79 and name HN  ) (residue 75  and name O )     1.80  0.0  0.40
assign (residue 79 and name N   ) (residue 75  and name O )     2.80  0.30 0.40

!assign (residue 80 and name HN  ) (residue 76  and name O )     1.80  0.0  0.40
!assign (residue 80 and name N   ) (residue 76  and name O )     2.80  0.30 0.40

assign (residue 81 and name HN  ) (residue 77  and name O )     1.80  0.0  0.40
assign (residue 81 and name N   ) (residue 77  and name O )     2.80  0.30 0.40

assign (residue 82 and name HN  ) (residue 78  and name O )     1.80  0.0  0.40
assign (residue 82 and name N   ) (residue 78  and name O )     2.80  0.30 0.40

!Helix C
assign (residue 102 and name HN  ) (residue 98 and name O )     1.80  0.0  0.40
assign (residue 102 and name N   ) (residue 98 and name O )     2.80  0.30 0.40

assign (residue 103 and name HN  ) (residue 99 and name O )     1.80  0.0  0.40
assign (residue 103 and name N   ) (residue 99 and name O )     2.80  0.30 0.40

assign (residue 104 and name HN  ) (residue 100 and name O )     1.80  0.0  0.40
assign (residue 104 and name N   ) (residue 100 and name O )     2.80  0.30 0.40

assign (residue 105 and name HN  ) (residue 101 and name O )     1.80  0.0  0.40
assign (residue 105 and name N   ) (residue 101 and name O )     2.80  0.30 0.40
```

Table 5

Atomic Structure Coordinates of the Free Form of the P/CAF Bromodomain

```
REMARK FILENAME="/bloch2/chris/BROMO_XPLOR_ARIA32/structures/it0/brd_187.pdb"
REMARK initial random number seed: 1.142876E+11
REMARK ------------------------------------------------------------
REMARK             overall,bonds,angles,impropers,vdw,noe,cdih
REMARK energies: 157.923, 9.30626, 73.1523, 0, 23.1019, 36.4277, 0.228429
REMARK ------------------------------------------------------------
REMARK          bonds,angles,impropers,noe,cdih
REMARK rms-dev.: 2.164156E-03,0.365411,$0.3111,1.418985E-02,0.263503
REMARK ------------------------------------------------------------
REMARK                noe,  cdih
REMARK violations.: 2, 0
REMARK ------------------------------------------------------------
REMARK DATE:29-Nov-98  06:51:33       created by user:
ATOM      1  CA  GLY     1      27.208  16.825  -6.349  1.00  0.00
ATOM      2  HA1 GLY     1      26.763  16.827  -5.365  1.00  0.00
ATOM      3  HA2 GLY     1      28.041  17.514  -6.157  1.00  0.00
ATOM      4  C   GLY     1      27.723  15.432  -6.650  1.00  0.00
ATOM      5  O   GLY     1      28.656  15.263  -7.435  1.00  0.00
ATOM      6  N   GLY     1      26.194  17.285  -7.337  1.00  0.00
ATOM      7  HT1 GLY     1      26.586  18.049  -7.923  1.00  0.00
ATOM      8  HT2 GLY     1      25.350  17.641  -6.843  1.00  0.00
ATOM      9  HT3 GLY     1      25.914  16.498  -7.955  1.00  0.00
ATOM     10  N   SER     2      27.113  14.431  -6.024  1.00  0.00
ATOM     11  HN  SER     2      26.376  14.629  -5.409  1.00  0.00
ATOM     12  CA  SER     2      27.516  13.044  -6.226  1.00  0.00
ATOM     13  HA  SER     2      28.481  13.047  -6.712  1.00  0.00
ATOM     14  CB  SER     2      27.636  12.329  -4.878  1.00  0.00
ATOM     15  HB1 SER     2      26.904  12.729  -4.193  1.00  0.00
ATOM     16  HB2 SER     2      27.462  11.273  -5.017  1.00  0.00
ATOM     17  OG  SER     2      28.927  12.508  -4.319  1.00  0.00
ATOM     18  HG  SER     2      29.571  12.014  -4.832  1.00  0.00
ATOM     19  C   SER     2      26.519  12.308  -7.114  1.00  0.00
ATOM     20  O   SER     2      25.320  12.288  -6.835  1.00  0.00
ATOM     21  N   HIS     3      27.022  11.698  -8.183  1.00  0.00
ATOM     22  HN  HIS     3      27.986  11.747  -8.353  1.00  0.00
ATOM     23  CA  HIS     3      26.173  10.955  -9.106  1.00  0.00
ATOM     24  HA  HIS     3      25.157  11.295  -8.967  1.00  0.00
ATOM     25  CB  HIS     3      26.594  11.222 -10.553  1.00  0.00
ATOM     26  HB1 HIS     3      26.616  12.288 -10.722  1.00  0.00
ATOM     27  HB2 HIS     3      27.581  10.814 -10.714  1.00  0.00
ATOM     28  CG  HIS     3      25.671  10.612 -11.561  1.00  0.00
ATOM     29  ND1 HIS     3      25.985  10.494 -12.900  1.00  0.00
ATOM     30  HD1 HIS     3      26.820  10.790 -13.320  1.00  0.00
ATOM     31  CD2 HIS     3      24.433  10.080 -11.420  1.00  0.00
ATOM     32  HD2 HIS     3      23.870  10.003 -10.501  1.00  0.00
ATOM     33  CE1 HIS     3      24.981   9.918 -13.537  1.00  0.00
ATOM     34  HE1 HIS     3      24.945   9.698 -14.596  1.00  0.00
ATOM     35  NE2 HIS     3      24.028   9.658 -12.662  1.00  0.00
ATOM     36  HE2 HIS     3      23.171   9.230 -12.868  1.00  0.00
ATOM     37  C   HIS     3      26.233   9.459  -8.817  1.00  0.00
ATOM     38  O   HIS     3      26.214   8.638  -9.734  1.00  0.00
ATOM     39  N   MET     4      26.305   9.111  -7.536  1.00  0.00
ATOM     40  HN  MET     4      26.314   9.811  -6.850  1.00  0.00
ATOM     41  CA  MET     4      26.364   7.713  -7.128  1.00  0.00
ATOM     42  HA  MET     4      26.164   7.105  -7.998  1.00  0.00
ATOM     43  CB  MET     4      27.755   7.374  -6.591  1.00  0.00
ATOM     44  HB1 MET     4      28.456   8.117  -6.944  1.00  0.00
ATOM     45  HB2 MET     4      27.730   7.400  -5.512  1.00  0.00
ATOM     46  CG  MET     4      28.294   6.005  -7.024  1.00  0.00
ATOM     47  HG1 MET     4      27.433   5.306  -6.972  1.00  0.00
ATOM     48  HG2 MET     4      28.606   6.071  -8.063  1.00  0.00
ATOM     49  SD  MET     4      29.597   5.394  -5.988  1.00  0.00
ATOM     50  CE  MET     4      28.922   3.825  -5.449  1.00  0.00
ATOM     51  HE1 MET     4      29.243   3.623  -4.438  1.00  0.00
ATOM     52  HE2 MET     4      29.273   3.039  -6.102  1.00  0.00
ATOM     53  HE3 MET     4      27.843   3.866  -5.483  1.00  0.00
ATOM     54  C   MET     4      25.310   7.413  -6.067  1.00  0.00
ATOM     55  O   MET     4      25.333   7.983  -4.977  1.00  0.00
ATOM     56  N   SER     5      24.386   6.517  -6.398  1.00  0.00
ATOM     57  HN  SER     5      24.422   6.098  -7.283  1.00  0.00
ATOM     58  CA  SER     5      23.321   6.141  -5.476  1.00  0.00
ATOM     59  HA  SER     5      23.780   5.750  -4.580  1.00  0.00
ATOM     60  CB  SER     5      22.479   7.366  -5.111  1.00  0.00
ATOM     61  HB1 SER     5      22.188   7.882  -6.014  1.00  0.00
ATOM     62  HB2 SER     5      23.062   8.029  -4.490  1.00  0.00
ATOM     63  OG  SER     5      21.309   6.990  -4.405  1.00  0.00
ATOM     64  HG  SER     5      21.060   7.693  -3.800  1.00  0.00
ATOM     65  C   SER     5      22.431   5.062  -6.084  1.00  0.00
ATOM     66  O   SER     5      21.471   5.362  -6.794  1.00  0.00
ATOM     67  N   LYS     6      22.756   3.805  -5.800  1.00  0.00
ATOM     68  HN  LYS     6      23.532   3.630  -5.228  1.00  0.00
ATOM     69  CA  LYS     6      21.987   2.680  -6.319  1.00  0.00
ATOM     70  HA  LYS     6      21.642   2.942  -7.308  1.00  0.00
ATOM     71  CB  LYS     6      22.869   1.433  -6.409  1.00  0.00
ATOM     72  HB1 LYS     6      22.266   0.563  -6.192  1.00  0.00
ATOM     73  HB2 LYS     6      23.655   1.508  -5.673  1.00  0.00
ATOM     74  CG  LYS     6      23.510   1.238  -7.773  1.00  0.00
ATOM     75  HG1 LYS     6      24.045   2.138  -8.041  1.00  0.00
ATOM     76  HG2 LYS     6      24.201   0.409  -7.721  1.00  0.00
ATOM     77  CD  LYS     6      22.469   0.947  -8.842  1.00  0.00
ATOM     78  HD1 LYS     6      21.794   1.787  -8.911  1.00  0.00
ATOM     79  HD2 LYS     6      22.970   0.804  -9.788  1.00  0.00
ATOM     80  CE  LYS     6      21.669  -0.304  -8.514  1.00  0.00
ATOM     81  HE1 LYS     6      21.107  -0.129  -7.608  1.00  0.00
ATOM     82  HE2 LYS     6      20.967  -0.503  -9.327  1.00  0.00
ATOM     83  NZ  LYS     6      22.548  -1.489  -8.317  1.00  0.00
ATOM     84  HZ1 LYS     6      23.320  -1.481  -9.014  1.00  0.00
ATOM     85  HZ2 LYS     6      21.999  -2.368  -8.435  1.00  0.00
ATOM     86  HZ3 LYS     6      22.958  -1.476  -7.362  1.00  0.00
ATOM     87  C   LYS     6      20.776   2.397  -5.436  1.00  0.00
ATOM     88  O   LYS     6      20.863   1.638  -4.471  1.00  0.00
ATOM     89  N   GLU     7      19.646   3.011  -5.773  1.00  0.00
ATOM     90  HN  GLU     7      19.637   3.606  -6.552  1.00  0.00
ATOM     91  CA  GLU     7      18.420   2.825  -5.005  1.00  0.00
ATOM     92  HA  GLU     7      18.531   1.926  -4.418  1.00  0.00
ATOM     93  CB  GLU     7      18.200   4.011  -4.064  1.00  0.00
ATOM     94  HB1 GLU     7      18.505   4.916  -4.567  1.00  0.00
ATOM     95  HB2 GLU     7      17.148   4.078  -3.828  1.00  0.00
ATOM     96  CG  GLU     7      18.975   3.904  -2.761  1.00  0.00
ATOM     97  HG1 GLU     7      19.746   3.156  -2.876  1.00  0.00
ATOM     98  HG2 GLU     7      19.430   4.860  -2.948  1.00  0.00
ATOM     99  CD  GLU     7      18.095   3.515  -1.589  1.00  0.00
ATOM    100  OE1 GLU     7      17.118   4.243  -1.312  1.00  0.00
ATOM    101  OE2 GLU     7      18.383   2.483  -0.947  1.00  0.00
ATOM    102  C   GLU     7      17.215   2.662  -5.928  1.00  0.00
ATOM    103  O   GLU     7      16.278   3.461  -5.886  1.00  0.00
ATOM    104  N   PRO     8      17.218   1.617  -6.772  1.00  0.00
ATOM    105  CA  PRO     8      16.120   1.352  -7.702  1.00  0.00
ATOM    106  HA  PRO     8      15.785   2.256  -8.189  1.00  0.00
ATOM    107  CB  PRO     8      16.760   0.419  -8.727  1.00  0.00
ATOM    108  HB1 PRO     8      17.200   1.002  -9.523  1.00  0.00
ATOM    109  HB2 PRO     8      16.011  -0.245  -9.130  1.00  0.00
ATOM    110  CG  PRO     8      17.796  -0.327  -7.958  1.00  0.00
ATOM    111  HG1 PRO     8      17.357  -1.205  -7.508  1.00  0.00
ATOM    112  HG2 PRO     8      18.607  -0.608  -8.614  1.00  0.00
ATOM    113  CD  PRO     8      18.294   0.613  -6.889  1.00  0.00
ATOM    114  HD1 PRO     8      18.429   0.085  -5.956  1.00  0.00
ATOM    115  HD2 PRO     8      19.220   1.076  -7.197  1.00  0.00
ATOM    116  C   PRO     8      14.938   0.669  -7.021  1.00  0.00
ATOM    117  O   PRO     8      13.782   0.924  -7.360  1.00  0.00
ATOM    118  N   ARG     9      15.236  -0.196  -6.057  1.00  0.00
ATOM    119  HN  ARG     9      16.176  -0.357  -5.833  1.00  0.00
ATOM    120  CA  ARG     9      14.199  -0.917  -5.328  1.00  0.00
ATOM    121  HA  ARG     9      13.522  -0.169  -4.906  1.00  0.00
ATOM    122  CB  ARG     9      13.421  -1.830  -6.279  1.00  0.00
ATOM    123  HB1 ARG     9      12.812  -2.504  -5.695  1.00  0.00
ATOM    124  HB2 ARG     9      12.778  -1.222  -6.898  1.00  0.00
ATOM    125  CG  ARG     9      14.313  -2.661  -7.188  1.00  0.00
ATOM    126  HG1 ARG     9      14.295  -2.236  -8.181  1.00  0.00
ATOM    127  HG2 ARG     9      15.322  -2.640  -6.803  1.00  0.00
ATOM    128  CD  ARG     9      13.843  -4.106  -7.262  1.00  0.00
ATOM    129  HD1 ARG     9      13.031  -4.518  -6.264  1.00  0.00
ATOM    130  HD2 ARG     9      12.844  -4.125  -7.671  1.00  0.00
ATOM    131  NE  ARG     9      14.714  -4.926  -8.102  1.00  0.00
ATOM    132  HE  ARG     9      15.302  -4.464  -8.735  1.00  0.00
ATOM    133  CZ  ARG     9      14.745  -6.255  -8.053  1.00  0.00
ATOM    134  NH1 ARG     9      13.960  -6.908  -7.208  1.00  0.00
ATOM    135 HH11 ARG     9      13.342  -6.401  -6.606  1.00  0.00
ATOM    136 HH12 ARG     9      13.985  -7.907  -7.172  1.00  0.00
ATOM    137  NH2 ARG     9      15.563  -6.932  -8.850  1.00  0.00
ATOM    138 HH21 ARG     9      16.157  -6.444  -9.489  1.00  0.00
ATOM    139 HH22 ARG     9      15.585  -7.931  -8.810  1.00  0.00
ATOM    140  C   ARG     9      14.800  -1.744  -4.196  1.00  0.00
ATOM    141  O   ARG     9      14.421  -2.897  -3.991  1.00  0.00
ATOM    142  N   ASP    10      15.732  -1.144  -3.450  1.00  0.00
ATOM    143  HN  ASP    10      15.988  -0.223  -3.673  1.00  0.00
ATOM    144  CA  ASP    10      16.393  -1.824  -2.345  1.00  0.00
ATOM    145  HA  ASP    10      17.087  -2.540  -2.760  1.00  0.00
ATOM    146  CB  ASP    10      17.169  -0.813  -1.497  1.00  0.00
ATOM    147  HB1 ASP    10      17.594  -0.061  -2.146  1.00  0.00
ATOM    148  HB2 ASP    10      16.490  -0.341  -0.802  1.00  0.00
ATOM    149  CG  ASP    10      18.292  -1.457  -0.708  1.00  0.00
ATOM    150  OD1 ASP    10      18.771  -2.532  -1.126  1.00  0.00
ATOM    151  OD2 ASP    10      18.692  -0.886   0.328  1.00  0.00
ATOM    152  C   ASP    10      15.383  -2.565  -1.468  1.00  0.00
ATOM    153  O   ASP    10      14.728  -1.961  -0.619  1.00  0.00
ATOM    154  N   PRO    11      15.249  -3.889  -1.658  1.00  0.00
ATOM    155  CA  PRO    11      14.309  -4.709  -0.867  1.00  0.00
ATOM    156  HA  PRO    11      13.311  -4.297  -0.920  1.00  0.00
ATOM    157  CB  PRO    11      14.326  -6.068  -1.607  1.00  0.00
ATOM    158  HB1 PRO    11      13.331  -6.399  -1.772  1.00  0.00
ATOM    159  HB2 PRO    11      14.849  -6.791  -0.999  1.00  0.00
ATOM    160  CG  PRO    11      15.036  -5.829  -2.899  1.00  0.00
ATOM    161  HG1 PRO    11      15.582  -6.715  -3.188  1.00  0.00
ATOM    162  HG2 PRO    11      14.324  -5.561  -3.666  1.00  0.00
ATOM    163  CD  PRO    11      15.981  -4.692  -2.646  1.00  0.00
ATOM    164  HD1 PRO    11      16.155  -4.133  -3.552  1.00  0.00
ATOM    165  HD2 PRO    11      16.911  -5.056  -2.237  1.00  0.00
ATOM    166  C   PRO    11      14.732  -4.881   0.572  1.00  0.00
ATOM    167  O   PRO    11      13.991  -5.446   1.375  1.00  0.00
ATOM    168  N   ASP    12      15.926  -4.397   0.912  1.00  0.00
ATOM    169  HN  ASP    12      16.477  -3.954   0.236  1.00  0.00
ATOM    170  CA  ASP    12      16.430  -4.508   2.276  1.00  0.00
ATOM    171  HA  ASP    12      16.402  -5.551   2.554  1.00  0.00
ATOM    172  CB  ASP    12      17.874  -4.008   2.352  1.00  0.00
ATOM    173  HB1 ASP    12      18.146  -3.873   3.389  1.00  0.00
ATOM    174  HB2 ASP    12      17.948  -3.061   1.839  1.00  0.00
ATOM    175  CG  ASP    12      18.856  -4.975   1.721  1.00  0.00
ATOM    176  OD1 ASP    12      18.870  -6.157   2.125  1.00  0.00
ATOM    177  OD2 ASP    12      19.615  -4.549   0.824  1.00  0.00
ATOM    178  C   ASP    12      15.555  -3.719   3.243  1.00  0.00
ATOM    179  O   ASP    12      14.689  -4.282   3.913  1.00  0.00
ATOM    180  N   GLN    13      15.785  -2.412   3.309  1.00  0.00
ATOM    181  HN  GLN    13      16.486  -2.020   2.748  1.00  0.00
ATOM    182  CA  GLN    13      15.012  -1.546   4.191  1.00  0.00
ATOM    183  HA  GLN    13      15.115  -1.923   5.197  1.00  0.00
ATOM    184  CB  GLN    13      15.550  -0.115   4.134  1.00  0.00
ATOM    185  HB1 GLN    13      15.055   0.411   3.331  1.00  0.00
ATOM    186  HB2 GLN    13      16.610  -0.149   3.931  1.00  0.00
ATOM    187  CG  GLN    13      15.336   0.669   5.420  1.00  0.00
ATOM    188  HG1 GLN    13      15.288  -0.025   6.246  1.00  0.00
ATOM    189  HG2 GLN    13      14.403   1.208   5.247  1.00  0.00
ATOM    190  CD  GLN    13      16.490   1.662   5.687  1.00  0.00
ATOM    191  OE1 GLN    13      16.878   2.391   4.790  1.00  0.00
ATOM    192  NE2 GLN    13      16.930   1.695   6.925  1.00  0.00
ATOM    193 HE21 GLN    13      17.651   2.328   7.125  1.00  0.00
ATOM    194 HE22 GLN    13      16.543   1.085   7.587  1.00  0.00
ATOM    195  C   GLN    13      13.538  -1.566   3.807  1.00  0.00
ATOM    196  O   GLN    13      12.658  -1.499   4.666  1.00  0.00
ATOM    197  N   LEU    14      13.278  -1.666   2.509  1.00  0.00
ATOM    198  HN  LEU    14      14.025  -1.723   1.877  1.00  0.00
ATOM    199  CA  LEU    14      11.914  -1.713   1.999  1.00  0.00
ATOM    200  HA  LEU    14      11.445  -0.764   2.212  1.00  0.00
ATOM    201  CB  LEU    14      11.939  -1.932   0.481  1.00  0.00
ATOM    202  HB1 LEU    14      12.218  -1.001   0.012  1.00  0.00
ATOM    203  HB2 LEU    14      12.702  -2.664   0.261  1.00  0.00
ATOM    204  CG  LEU    14      10.625  -2.407  -0.145  1.00  0.00
ATOM    205  HG  LEU    14       9.801  -1.900   0.133  1.00  0.00
ATOM    206  CD1 LEU    14      10.592  -2.066  -1.628  1.00  0.00
ATOM    207 HD11 LEU    14      11.506  -2.403  -2.095  1.00  0.00
ATOM    208 HD12 LEU    14      10.499  -0.997  -1.749  1.00  0.00
ATOM    209 HD13 LEU    14       9.749  -2.556  -2.091  1.00  0.00
ATOM    210  CD2 LEU    14      10.444  -3.902   0.066  1.00  0.00
ATOM    211 HD21 LEU    14      11.402  -4.354   0.275  1.00  0.00
ATOM    212 HD22 LEU    14      10.026  -4.344  -0.828  1.00  0.00
ATOM    213 HD23 LEU    14       9.777  -4.071   0.897  1.00  0.00
ATOM    214  C   LEU    14      11.121  -2.822   2.688  1.00  0.00
ATOM    215  O   LEU    14      10.019  -2.595   3.188  1.00  0.00
ATOM    216  N   TYR    15      11.697  -4.018   2.715  1.00  0.00
ATOM    217  HN  TYR    15      12.579  -4.131   2.303  1.00  0.00
ATOM    218  CA  TYR    15      11.061  -5.167   3.350  1.00  0.00
ATOM    219  HA  TYR    15      10.125  -5.357   2.843  1.00  0.00
ATOM    220  CB  TYR    15      11.964  -6.394   3.218  1.00  0.00
ATOM    221  HB1 TYR    15      12.163  -6.569   2.173  1.00  0.00
ATOM    222  HB2 TYR    15      12.896  -6.200   3.728  1.00  0.00
ATOM    223  CG  TYR    15      11.374  -7.659   3.798  1.00  0.00
ATOM    224  CD1 TYR    15      12.076  -8.408   4.734  1.00  0.00
ATOM    225  HD1 TYR    15      13.051  -8.070   5.053  1.00  0.00
ATOM    226  CD2 TYR    15      10.121  -8.111   3.402  1.00  0.00
ATOM    227  HD2 TYR    15       9.564  -7.543   2.671  1.00  0.00
ATOM    228  CE1 TYR    15      11.542  -9.565   5.268  1.00  0.00
ATOM    229  HE1 TYR    15      12.102 -10.132   5.998  1.00  0.00
ATOM    230  CE2 TYR    15       9.582  -9.269   3.929  1.00  0.00
ATOM    231  HE2 TYR    15       8.606  -9.604   3.610  1.00  0.00
ATOM    232  CZ  TYR    15      10.296  -9.993   4.860  1.00  0.00
ATOM    233  OH  TYR    15       9.761 -11.145   5.388  1.00  0.00
ATOM    234  HH  TYR    15      10.392 -11.863   5.295  1.00  0.00
ATOM    235  C   TYR    15      10.776  -4.888   4.821  1.00  0.00
ATOM    236  O   TYR    15       9.750  -5.307   5.356  1.00  0.00
ATOM    237  N   SER    16      11.694  -4.181   5.471  1.00  0.00
ATOM    238  HN  SER    16      12.487  -3.869   4.989  1.00  0.00
ATOM    239  CA  SER    16      11.525  -3.836   6.878  1.00  0.00
ATOM    240  HA  SER    16      11.318  -4.746   7.420  1.00  0.00
ATOM    241  CB  SER    16      12.824  -3.220   7.425  1.00  0.00
ATOM    242  HB1 SER    16      13.672  -3.768   7.042  1.00  0.00
ATOM    243  HB2 SER    16      12.889  -2.189   7.111  1.00  0.00
ATOM    244  OG  SER    16      12.852  -3.268   8.841  1.00  0.00
ATOM    245  HG  SER    16      13.743  -3.471   9.137  1.00  0.00
ATOM    246  C   SER    16      10.373  -2.867   7.061  1.00  0.00
ATOM    247  O   SER    16       9.746  -2.824   8.120  1.00  0.00
ATOM    248  N   THR    17      10.067  -2.096   6.017  1.00  0.00
ATOM    249  HN  THR    17      10.615  -2.189   5.195  1.00  0.00
ATOM    250  CA  THR    17       8.983  -1.146   6.049  1.00  0.00
ATOM    251  HA  THR    17       8.965  -0.685   7.025  1.00  0.00
ATOM    252  CB  THR    17       9.182  -0.061   4.982  1.00  0.00
ATOM    253  HB  THR    17       9.395  -0.537   4.037  1.00  0.00
ATOM    254  OG1 THR    17      10.278   0.771   5.316  1.00  0.00
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ATOM    255  HG1 THR  17      10.098   1.223   6.144  1.00  0.00
ATOM    256  CG2 THR  17       7.971   0.832   4.783  1.00  0.00
ATOM    257 HG21 THR  17       7.078   0.224   4.720  1.00  0.00
ATOM    258 HG22 THR  17       8.088   1.395   3.867  1.00  0.00
ATOM    259 HG23 THR  17       7.883   1.513   5.616  1.00  0.00
ATOM    260  C   THR  17       7.662  -1.866   5.821  1.00  0.00
ATOM    261  O   THR  17       6.756  -1.792   6.646  1.00  0.00
ATOM    262  N   LEU  18       7.576  -2.569   4.697  1.00  0.00
ATOM    263  HN  LEU  18       8.339  -2.578   4.083  1.00  0.00
ATOM    264  CA  LEU  18       6.369  -3.302   4.330  1.00  0.00
ATOM    265  HA  LEU  18       5.555  -2.597   4.289  1.00  0.00
ATOM    266  CB  LEU  18       6.550  -3.928   2.955  1.00  0.00
ATOM    267  HB1 LEU  18       7.307  -4.694   3.026  1.00  0.00
ATOM    268  HB2 LEU  18       5.619  -4.389   2.661  1.00  0.00
ATOM    269  CG  LEU  18       6.964  -2.840   1.675  1.00  0.00
ATOM    270  HG  LEU  18       7.969  -2.603   2.075  1.00  0.00
ATOM    271  CD1 LEU  18       6.954  -3.607   0.510  1.00  0.00
ATOM    272 HD11 LEU  18       7.945  -3.963   0.274  1.00  0.00
ATOM    273 HD12 LEU  18       6.640  -2.894  -0.236  1.00  0.00
ATOM    274 HD13 LEU  18       6.270  -4.442   0.524  1.00  0.00
ATOM    275  CD2 LEU  18       6.048  -1.722   1.899  1.00  0.00
ATOM    276 HD21 LEU  18       5.138  -1.963   2.430  1.00  0.00
ATOM    277 HD22 LEU  18       5.811  -1.428   0.889  1.00  0.00
ATOM    278 HD23 LEU  18       6.549  -0.908   2.401  1.00  0.00
ATOM    279  C   LEU  18       6.037  -4.376   5.349  1.00  0.00
ATOM    280  O   LEU  18       4.961  -4.372   5.942  1.00  0.00
ATOM    281  N   LYS  19       6.956  -5.310   5.541  1.00  0.00
ATOM    282  HN  LYS  19       7.802  -5.262   5.048  1.00  0.00
ATOM    283  CA  LYS  19       6.783  -6.372   6.514  1.00  0.00
ATOM    284  HA  LYS  19       5.946  -6.995   6.158  1.00  0.00
ATOM    285  CB  LYS  19       8.029  -7.225   6.635  1.00  0.00
ATOM    286  HB1 LYS  19       8.522  -7.243   5.674  1.00  0.00
ATOM    287  HB2 LYS  19       7.748  -8.232   6.897  1.00  0.00
ATOM    288  CG  LYS  19       9.033  -6.730   7.669  1.00  0.00
ATOM    289  HG1 LYS  19       8.693  -7.018   8.653  1.00  0.00
ATOM    290  HG2 LYS  19       9.096  -5.653   7.608  1.00  0.00
ATOM    291  CD  LYS  19      10.412  -7.319   7.429  1.00  0.00
ATOM    292  HD1 LYS  19      10.559  -7.440   6.365  1.00  0.00
ATOM    293  HD2 LYS  19      11.156  -6.643   7.823  1.00  0.00
ATOM    294  CE  LYS  19      10.567  -8.671   8.106  1.00  0.00
ATOM    295  HE1 LYS  19       9.987  -9.401   7.560  1.00  0.00
ATOM    296  HE2 LYS  19      10.193  -8.598   9.117  1.00  0.00
ATOM    297  NZ  LYS  19      11.988  -9.115   8.146  1.00  0.00
ATOM    298  HZ1 LYS  19      12.044 -10.147   8.030  1.00  0.00
ATOM    299  HZ2 LYS  19      12.418  -8.855   9.057  1.00  0.00
ATOM    300  HZ3 LYS  19      12.526  -8.661   7.380  1.00  0.00
ATOM    301  C   LYS  19       6.349  -5.772   7.863  1.00  0.00
ATOM    302  O   LYS  19       5.624  -6.390   8.646  1.00  0.00
ATOM    303  N   SER  20       6.797  -4.542   8.100  1.00  0.00
ATOM    304  HN  SER  20       7.346  -4.092   7.419  1.00  0.00
ATOM    305  CA  SER  20       6.482  -3.841   9.336  1.00  0.00
ATOM    306  HA  SER  20       6.548  -4.551  10.141  1.00  0.00
ATOM    307  CB  SER  20       7.481  -2.708   9.581  1.00  0.00
ATOM    308  HB1 SER  20       7.647  -2.171   8.659  1.00  0.00
ATOM    309  HB2 SER  20       8.416  -3.123   9.929  1.00  0.00
ATOM    310  OG  SER  20       6.996  -1.801  10.556  1.00  0.00
ATOM    311  HG  SER  20       7.552  -1.841  11.337  1.00  0.00
ATOM    312  C   SER  20       5.070  -3.288   9.292  1.00  0.00
ATOM    313  O   SER  20       4.188  -3.752  10.016  1.00  0.00
ATOM    314  N   ILE  21       4.851  -2.311   8.423  1.00  0.00
ATOM    315  HN  ILE  21       5.590  -1.989   7.866  1.00  0.00
ATOM    316  CA  ILE  21       3.531  -1.717   8.268  1.00  0.00
ATOM    317  HA  ILE  21       3.312  -1.154   9.164  1.00  0.00
ATOM    318  CB  ILE  21       3.477  -0.752   7.069  1.00  0.00
ATOM    319  HB  ILE  21       2.442  -0.564   6.839  1.00  0.00
ATOM    320 CG1 ILE  21       4.155  -1.368   5.846  1.00  0.00
ATOM    321 HG11 ILE  21       4.819  -0.640   5.404  1.00  0.00
ATOM    322 HG12 ILE  21       4.723  -2.227   6.152  1.00  0.00
ATOM    323 CG2 ILE  21       4.130   0.573   7.427  1.00  0.00
ATOM    324 HG21 ILE  21       3.498   1.385   7.101  1.00  0.00
ATOM    325 HG22 ILE  21       5.089   0.644   6.935  1.00  0.00
ATOM    326 HG23 ILE  21       4.268   0.630   8.496  1.00  0.00
ATOM    327  CD1 ILE  21       3.185  -1.819   4.782  1.00  0.00
ATOM    328 HD11 ILE  21       2.645  -2.684   5.134  1.00  0.00
ATOM    329 HD12 ILE  21       3.729  -2.074   3.885  1.00  0.00
ATOM    330 HD13 ILE  21       2.489  -1.022   4.568  1.00  0.00
ATOM    331  C   ILE  21       2.472  -2.801   8.095  1.00  0.00
ATOM    332  O   ILE  21       1.447  -2.838   8.823  1.00  0.00
ATOM    333  N   LEU  22       2.710  -3.715   7.164  1.00  0.00
ATOM    334  HN  LEU  22       3.520  -3.646   6.622  1.00  0.00
ATOM    335  CA  LEU  22       1.785  -4.812   6.920  1.00  0.00
ATOM    336  HA  LEU  22       0.864  -4.390   6.544  1.00  0.00
ATOM    337  CB  LEU  22       2.361  -5.772   5.874  1.00  0.00
ATOM    338  HB1 LEU  22       1.785  -6.685   5.900  1.00  0.00
ATOM    339  HB2 LEU  22       3.379  -6.000   6.147  1.00  0.00
ATOM    340  CG  LEU  22       2.360  -5.245   4.439  1.00  0.00
ATOM    341  HG  LEU  22       3.054  -4.421   4.365  1.00  0.00
ATOM    342 CD1 LEU  22       2.815  -6.329   3.474  1.00  0.00
ATOM    343 HD11 LEU  22       2.102  -6.416   2.668  1.00  0.00
ATOM    344 HD12 LEU  22       2.885  -7.271   3.997  1.00  0.00
ATOM    345 HD13 LEU  22       3.783  -6.069   3.071  1.00  0.00
ATOM    346 CD2 LEU  22       0.980  -4.733   4.057  1.00  0.00
ATOM    347 HD21 LEU  22       0.926  -3.671   4.243  1.00  0.00
ATOM    348 HD22 LEU  22       0.234  -5.242   4.647  1.00  0.00
ATOM    349 HD23 LEU  22       0.803  -4.924   3.008  1.00  0.00
ATOM    350  C   LEU  22       1.493  -5.568   8.214  1.00  0.00
ATOM    351  O   LEU  22       0.340  -5.862   8.525  1.00  0.00
ATOM    352  N   GLN  23       2.546  -5.868   8.971  1.00  0.00
ATOM    353  HN  GLN  23       3.447  -5.617   8.666  1.00  0.00
ATOM    354  CA  GLN  23       2.402  -6.598  10.226  1.00  0.00
ATOM    355  HA  GLN  23       2.066  -7.596   9.989  1.00  0.00
ATOM    356  CB  GLN  23       3.754  -6.684  10.940  1.00  0.00
ATOM    357  HB1 GLN  23       3.588  -6.635  12.006  1.00  0.00
ATOM    358  HB2 GLN  23       4.360  -5.842  10.640  1.00  0.00
ATOM    359  CG  GLN  23       4.528  -7.958  10.637  1.00  0.00
ATOM    360  HG1 GLN  23       4.592  -8.082   9.566  1.00  0.00
ATOM    361  HG2 GLN  23       5.523  -7.865  11.048  1.00  0.00
ATOM    362  CD  GLN  23       3.875  -9.191  11.231  1.00  0.00
ATOM    363  OE1 GLN  23       3.304  -9.141  12.320  1.00  0.00
ATOM    364  NE2 GLN  23       3.958 -10.308  10.517  1.00  0.00
ATOM    365 HE21 GLN  23       3.545 -11.120  10.879  1.00  0.00
ATOM    366 HE22 GLN  23       4.429 -10.275   9.658  1.00  0.00
ATOM    367  C   GLN  23       1.374  -5.941  11.151  1.00  0.00
ATOM    368  O   GLN  23       0.462  -6.604  11.646  1.00  0.00
ATOM    369  N   GLN  24       1.542  -4.645  11.404  1.00  0.00
ATOM    370  HN  GLN  24       2.303  -4.175  11.002  1.00  0.00
ATOM    371  CA  GLN  24       0.659  -3.920  12.317  1.00  0.00
ATOM    372  HA  GLN  24       0.414  -4.560  13.142  1.00  0.00
ATOM    373  CB  GLN  24       1.369  -2.679  12.863  1.00  0.00
ATOM    374  HB1 GLN  24       2.330  -2.973  13.260  1.00  0.00
ATOM    375  HB2 GLN  24       0.774  -2.258  13.659  1.00  0.00
ATOM    376  CG  GLN  24       1.596  -1.602  11.817  1.00  0.00
ATOM    377  HG1 GLN  24       0.680  -1.044  11.689  1.00  0.00
ATOM    378  HG2 GLN  24       1.860  -2.077  10.885  1.00  0.00
ATOM    379  CD  GLN  24       2.702  -0.638  12.200  1.00  0.00
ATOM    380  OE1 GLN  24       3.210  -0.671  13.320  1.00  0.00
ATOM    381  NE2 GLN  24       3.082   0.227  11.266  1.00  0.00
ATOM    382 HE21 GLN  24       2.633   0.195  10.395  1.00  0.00
ATOM    383 HE22 GLN  24       3.795   0.862  11.486  1.00  0.00
ATOM    384  C   GLN  24      -0.658  -3.511  11.654  1.00  0.00
ATOM    385  O   GLN  24      -1.727  -3.682  12.237  1.00  0.00
ATOM    386  N   VAL  25      -0.577  -2.936  10.456  1.00  0.00
ATOM    387  HN  VAL  25       0.298  -2.811  10.047  1.00  0.00
ATOM    388  CA  VAL  25      -1.769  -2.477   9.743  1.00  0.00
ATOM    389  HA  VAL  25      -2.139  -1.597  10.251  1.00  0.00
ATOM    390  CB  VAL  25      -1.454  -2.088   8.285  1.00  0.00
ATOM    391  HB  VAL  25      -2.344  -1.670   7.845  1.00  0.00
ATOM    392 CG1 VAL  25      -0.364  -1.025   8.239  1.00  0.00
ATOM    393 HG11 VAL  25      -0.774  -0.102   7.858  1.00  0.00
ATOM    394 HG12 VAL  25       0.434  -1.358   7.591  1.00  0.00
ATOM    395 HG13 VAL  25       0.026  -0.863   9.234  1.00  0.00
ATOM    396 CG2 VAL  25      -1.061  -3.301   7.473  1.00  0.00
ATOM    397 HG21 VAL  25      -1.924  -3.934   7.330  1.00  0.00
ATOM    398 HG22 VAL  25      -0.295  -3.848   7.997  1.00  0.00
ATOM    399 HG23 VAL  25      -0.684  -2.982   6.511  1.00  0.00
ATOM    400  C   VAL  25      -2.865  -3.536   9.760  1.00  0.00
ATOM    401  O   VAL  25      -4.042  -3.213   9.907  1.00  0.00
ATOM    402  N   LYS  26      -2.478  -4.805   9.670  1.00  0.00
ATOM    403  HN  LYS  26      -1.525  -5.013   9.579  1.00  0.00
ATOM    404  CA  LYS  26      -3.448  -5.893   9.728  1.00  0.00
ATOM    405  HA  LYS  26      -4.076  -5.827   8.852  1.00  0.00
ATOM    406  CB  LYS  26      -2.739  -7.248   9.740  1.00  0.00
ATOM    407  HB1 LYS  26      -2.064  -7.280  10.582  1.00  0.00
ATOM    408  HB2 LYS  26      -3.479  -8.026   9.853  1.00  0.00
ATOM    409  CG  LYS  26      -1.940  -7.530   8.479  1.00  0.00
ATOM    410  HG1 LYS  26      -2.552  -8.102   7.797  1.00  0.00
ATOM    411  HG2 LYS  26      -1.665  -6.591   8.020  1.00  0.00
ATOM    412  CD  LYS  26      -0.679  -8.317   8.790  1.00  0.00
ATOM    413  HD1 LYS  26      -0.295  -7.995   9.747  1.00  0.00
ATOM    414  HD2 LYS  26       0.054  -8.123   8.020  1.00  0.00
ATOM    415  CE  LYS  26      -0.955  -9.811   8.844  1.00  0.00
ATOM    416  HE1 LYS  26      -0.358 -10.245   9.632  1.00  0.00
ATOM    417  HE2 LYS  26      -2.002  -9.962   9.062  1.00  0.00
ATOM    418  NZ  LYS  26      -0.625 -10.486   7.558  1.00  0.00
ATOM    419  HZ1 LYS  26       0.302 -10.951   7.627  1.00  0.00
ATOM    420  HZ2 LYS  26      -0.595  -9.790   6.787  1.00  0.00
ATOM    421  HZ3 LYS  26      -1.345 -11.203   7.336  1.00  0.00
ATOM    422  C   LYS  26      -4.318  -5.750  10.973  1.00  0.00
ATOM    423  O   LYS  26      -5.496  -6.105  10.969  1.00  0.00
ATOM    424  N   SER  27      -3.724  -5.203  12.029  1.00  0.00
ATOM    425  HN  SER  27      -2.783  -4.928  11.957  1.00  0.00
ATOM    426  CA  SER  27      -4.437  -4.970  13.281  1.00  0.00
ATOM    427  HA  SER  27      -5.407  -5.436  13.209  1.00  0.00
ATOM    428  CB  SER  27      -3.669  -5.585  14.452  1.00  0.00
ATOM    429  HB1 SER  27      -2.861  -4.927  14.735  1.00  0.00
ATOM    430  HB2 SER  27      -3.267  -6.542  14.152  1.00  0.00
ATOM    431  OG  SER  27      -4.514  -5.777  15.573  1.00  0.00
ATOM    432  HG  SER  27      -5.402  -5.986  15.273  1.00  0.00
ATOM    433  C   SER  27      -4.643  -3.481  13.519  1.00  0.00
ATOM    434  O   SER  27      -4.887  -3.082  14.646  1.00  0.00
ATOM    435  N   HIS  28      -4.516  -2.692  12.457  1.00  0.00
ATOM    436  HN  HIS  28      -4.367  -3.088  11.578  1.00  0.00
ATOM    437  CA  HIS  28      -4.755  -1.267  12.552  1.00  0.00
ATOM    438  HA  HIS  28      -4.393  -0.936  13.515  1.00  0.00
ATOM    439  CB  HIS  28      -4.006  -0.512  11.456  1.00  0.00
ATOM    440  HB1 HIS  28      -2.948  -0.628  11.622  1.00  0.00
ATOM    441  HB2 HIS  28      -4.266  -0.930  10.496  1.00  0.00
ATOM    442  CG  HIS  28      -4.292   0.956  11.417  1.00  0.00
ATOM    443  ND1 HIS  28      -4.264   1.759  12.538  1.00  0.00
ATOM    444  HD1 HIS  28      -4.083   1.459  13.454  1.00  0.00
ATOM    445  CD2 HIS  28      -4.569   1.777  10.377  1.00  0.00
ATOM    446  HD2 HIS  28      -4.665   1.487   9.340  1.00  0.00
ATOM    447  CE1 HIS  28      -4.533   3.006  12.191  1.00  0.00
ATOM    448  HE1 HIS  28      -4.587   3.852  12.859  1.00  0.00
ATOM    449  NE2 HIS  28      -4.719   3.042  10.886  1.00  0.00
ATOM    450  HE2 HIS  28      -4.935   3.844  10.367  1.00  0.00
ATOM    451  C   HIS  28      -6.246  -1.009  12.480  1.00  0.00
ATOM    452  O   HIS  28      -6.982  -1.724  11.800  1.00  0.00
ATOM    453  N   GLN  29      -6.690  -0.037  13.241  1.00  0.00
ATOM    454  HN  GLN  29      -6.048   0.472  13.779  1.00  0.00
ATOM    455  CA  GLN  29      -8.109   0.272  13.334  1.00  0.00
ATOM    456  HA  GLN  29      -8.640  -0.668  13.358  1.00  0.00
ATOM    457  CB  GLN  29      -8.371   1.007  14.638  1.00  0.00
ATOM    458  HB1 GLN  29      -9.433   1.018  14.832  1.00  0.00
ATOM    459  HB2 GLN  29      -8.012   2.021  14.552  1.00  0.00
ATOM    460  CG  GLN  29      -7.670   0.341  15.809  1.00  0.00
ATOM    461  HG1 GLN  29      -7.180  -0.560  15.445  1.00  0.00
ATOM    462  HG2 GLN  29      -6.929   1.021  16.203  1.00  0.00
ATOM    463  CD  GLN  29      -8.622  -0.040  16.925  1.00  0.00
ATOM    464  OE1 GLN  29      -8.364   0.234  18.097  1.00  0.00
ATOM    465  NE2 GLN  29      -9.730  -0.676  16.566  1.00  0.00
ATOM    466 HE21 GLN  29      -9.870  -0.861  15.613  1.00  0.00
ATOM    467 HE22 GLN  29     -10.363  -0.935  17.267  1.00  0.00
ATOM    468  C   GLN  29      -8.607   1.069  12.132  1.00  0.00
ATOM    469  O   GLN  29      -9.794   1.378  12.034  1.00  0.00
ATOM    470  N   SER  30      -7.711   1.348  11.191  1.00  0.00
ATOM    471  HN  SER  30      -6.785   1.056  11.306  1.00  0.00
ATOM    472  CA  SER  30      -8.082   2.036   9.965  1.00  0.00
ATOM    473  HA  SER  30      -9.149   2.199   9.989  1.00  0.00
ATOM    474  CB  SER  30      -7.375   3.385   9.874  1.00  0.00
ATOM    475  HB1 SER  30      -6.453   3.269   9.324  1.00  0.00
ATOM    476  HB2 SER  30      -8.013   4.090   9.362  1.00  0.00
ATOM    477  OG  SER  30      -7.079   3.891  11.163  1.00  0.00
ATOM    478  HG  SER  30      -7.871   3.670  11.705  1.00  0.00
ATOM    479  C   SER  30      -7.743   1.184   8.740  1.00  0.00
ATOM    480  O   SER  30      -8.056   1.562   7.611  1.00  0.00
ATOM    481  N   ALA  31      -7.089   0.039   8.962  1.00  0.00
ATOM    482  HN  ALA  31      -6.867  -0.224   9.880  1.00  0.00
ATOM    483  CA  ALA  31      -6.726  -0.855   7.868  1.00  0.00
ATOM    484  HA  ALA  31      -6.413  -0.246   7.034  1.00  0.00
ATOM    485  CB  ALA  31      -5.553  -1.732   8.272  1.00  0.00
ATOM    486  HB1 ALA  31      -5.218  -2.301   7.417  1.00  0.00
ATOM    487  HB2 ALA  31      -5.865  -2.407   9.054  1.00  0.00
ATOM    488  HB3 ALA  31      -4.746  -1.111   8.629  1.00  0.00
ATOM    489  C   ALA  31      -7.906  -1.726   7.433  1.00  0.00
ATOM    490  O   ALA  31      -7.795  -2.496   6.480  1.00  0.00
ATOM    491  N   TRP  32      -9.040  -1.590   8.119  1.00  0.00
ATOM    492  HN  TRP  32      -9.072  -0.974   8.879  1.00  0.00
ATOM    493  CA  TRP  32     -10.222  -2.384   7.799  1.00  0.00
ATOM    494  HA  TRP  32      -9.960  -3.416   7.971  1.00  0.00
ATOM    495  CB  TRP  32     -11.389  -2.030   8.716  1.00  0.00
ATOM    496  HB1 TRP  32     -11.167  -2.390   9.720  1.00  0.00
ATOM    497  HB2 TRP  32     -12.289  -2.507   8.377  1.00  0.00
ATOM    498  CG  TRP  32     -11.644  -0.566   8.823  1.00  0.00
ATOM    499  CD1 TRP  32     -11.330   0.268   9.857  1.00  0.00
ATOM    500  HD1 TRP  32     -10.862  -0.052  10.776  1.00  0.00
ATOM    501  CD2 TRP  32     -12.255   0.241   7.823  1.00  0.00
ATOM    502  NE1 TRP  32     -11.699   1.554   9.549  1.00  0.00
ATOM    503  HE1 TRP  32     -11.582   2.335  10.128  1.00  0.00
ATOM    504  CE2 TRP  32     -12.259   1.564   8.298  1.00  0.00
ATOM    505  CE3 TRP  32     -12.759  -0.025   6.552  1.00  0.00
ATOM    506  HE3 TRP  32     -12.751  -1.026   6.146  1.00  0.00
ATOM    507  CZ2 TRP  32     -12.780   2.612   7.553  1.00  0.00
ATOM    508  HZ2 TRP  32     -12.798   3.627   7.923  1.00  0.00
ATOM    509  CZ3 TRP  32     -13.278   1.012   5.816  1.00  0.00
ATOM    510  HZ3 TRP  32     -13.671   0.827   4.829  1.00  0.00
ATOM    511  CH2 TRP  32     -13.284   2.314   6.317  1.00  0.00
ATOM    512  HH2 TRP  32     -13.669   3.090   5.697  1.00  0.00
ATOM    513  C   TRP  32     -10.647  -2.251   6.321  1.00  0.00
ATOM    514  O   TRP  32     -11.197  -3.202   5.769  1.00  0.00
ATOM    515  N   PRO  33     -10.400  -1.102   5.633  1.00  0.00
ATOM    516  CA  PRO  33     -10.776  -0.964   4.229  1.00  0.00
ATOM    517  HA  PRO  33     -11.746  -1.400   4.038  1.00  0.00
ATOM    518  CB  PRO  33     -10.842   0.550   3.996  1.00  0.00
ATOM    519  HB1 PRO  33     -10.273   0.798   3.113  1.00  0.00
ATOM    520  HB2 PRO  33     -11.870   0.844   3.852  1.00  0.00
ATOM    521  CG  PRO  33     -10.257   1.205   5.213  1.00  0.00
ATOM    522  HG1 PRO  33      -9.438   1.839   4.913  1.00  0.00
ATOM    523  HG2 PRO  33     -11.008   1.791   5.713  1.00  0.00
ATOM    524  CD  PRO  33      -9.749   0.125   6.125  1.00  0.00
ATOM    525  HD1 PRO  33      -8.693   0.063   6.031  1.00  0.00
ATOM    526  HD2 PRO  33     -10.014   0.330   7.146  1.00  0.00
ATOM    527  C   PRO  33      -9.748  -1.604   3.299  1.00  0.00
ATOM    528  O   PRO  33     -10.097  -2.161   2.259  1.00  0.00
ATOM    529  N   PHE  34      -8.481  -1.522   3.688  1.00  0.00
ATOM    530  HN  PHE  34      -8.271  -1.075   4.533  1.00  0.00
ATOM    531  CA  PHE  34      -7.393  -2.109   2.910  1.00  0.00
ATOM    532  HA  PHE  34      -7.546  -1.870   1.872  1.00  0.00
ATOM    533  CB  PHE  34      -6.043  -1.529   3.344  1.00  0.00
ATOM    534  HB1 PHE  34      -5.395  -1.497   2.486  1.00  0.00
ATOM    535  HB2 PHE  34      -5.608  -2.168   4.098  1.00  0.00
ATOM    536  CG  PHE  34      -6.120  -0.134   3.900  1.00  0.00
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ATOM    537  CD1 PHE  34      -6.997   0.794   3.361  1.00  0.00
ATOM    538  HD1 PHE  34      -7.638   0.503   2.542  1.00  0.00
ATOM    539  CD2 PHE  34      -5.300   0.255   4.946  1.00  0.00
ATOM    540  HD2 PHE  34      -4.611  -0.459   5.373  1.00  0.00
ATOM    541  CE1 PHE  34      -7.069   2.077   3.868  1.00  0.00
ATOM    542  HE1 PHE  34      -7.761   2.789   3.443  1.00  0.00
ATOM    543  CE2 PHE  34      -5.368   1.536   5.459  1.00  0.00
ATOM    544  HE2 PHE  34      -4.728   1.826   6.279  1.00  0.00
ATOM    545  CZ  PHE  34      -6.252   2.450   4.917  1.00  0.00
ATOM    546  HZ  PHE  34      -6.304   3.453   5.314  1.00  0.00
ATOM    547  C   PHE  34      -7.400  -3.624   3.053  1.00  0.00
ATOM    548  O   PHE  34      -7.293  -4.349   2.065  1.00  0.00
ATOM    549  N   MET  35      -7.543  -4.100   4.285  1.00  0.00
ATOM    550  HN  MET  35      -7.635  -3.476   5.035  1.00  0.00
ATOM    551  CA  MET  35      -7.587  -5.534   4.541  1.00  0.00
ATOM    552  HA  MET  35      -6.624  -5.948   4.283  1.00  0.00
ATOM    553  CB  MET  35      -7.868  -5.802   6.021  1.00  0.00
ATOM    554  HB1 MET  35      -8.472  -4.998   6.413  1.00  0.00
ATOM    555  HB2 MET  35      -8.415  -6.729   6.110  1.00  0.00
ATOM    556  CG  MET  35      -6.609  -5.910   6.868  1.00  0.00
ATOM    557  HG1 MET  35      -6.714  -5.267   7.730  1.00  0.00
ATOM    558  HG2 MET  35      -5.766  -5.582   6.278  1.00  0.00
ATOM    559  SD  MET  35      -6.296  -7.591   7.437  1.00  0.00
ATOM    560  CE  MET  35      -4.848  -8.011   6.470  1.00  0.00
ATOM    561  HE1 MET  35      -4.268  -8.726   7.013  1.00  0.00
ATOM    562  HE2 MET  35      -4.268  -7.119   6.285  1.00  0.00
ATOM    563  HE3 MET  35      -5.157  -8.441   5.529  1.00  0.00
ATOM    564  C   MET  35      -8.656  -6.194   3.674  1.00  0.00
ATOM    565  O   MET  35      -9.847  -5.924   3.827  1.00  0.00
ATOM    566  N   GLU  36      -8.219  -7.049   2.751  1.00  0.00
ATOM    567  HN  GLU  36      -7.255  -7.208   2.671  1.00  0.00
ATOM    568  CA  GLU  36      -9.128  -7.729   1.829  1.00  0.00
ATOM    569  HA  GLU  36      -8.598  -8.569   1.409  1.00  0.00
ATOM    570  CB  GLU  36     -10.371  -8.248   2.562  1.00  0.00
ATOM    571  HB1 GLU  36     -11.151  -7.504   2.496  1.00  0.00
ATOM    572  HB2 GLU  36     -10.122  -8.406   3.601  1.00  0.00
ATOM    573  CG  GLU  36     -10.907  -9.553   1.996  1.00  0.00
ATOM    574  HG1 GLU  36     -10.073 -10.192   1.748  1.00  0.00
ATOM    575  HG2 GLU  36     -11.673  -9.338   1.102  1.00  0.00
ATOM    576  CD  GLU  36     -11.806 -10.289   2.972  1.00  0.00
ATOM    577  OE1 GLU  36     -11.522 -11.469   3.266  1.00  0.00
ATOM    578  OE2 GLU  36     -12.794  -9.685   3.440  1.00  0.00
ATOM    579  C   GLU  36      -9.543  -6.792   0.696  1.00  0.00
ATOM    580  O   GLU  36     -10.414  -5.939   0.873  1.00  0.00
ATOM    581  N   PRO  37      -8.913  -6.929  -0.486  1.00  0.00
ATOM    582  CA  PRO  37      -9.200  -6.075  -1.644  1.00  0.00
ATOM    583  HA  PRO  37      -9.135  -5.029  -1.386  1.00  0.00
ATOM    584  CB  PRO  37      -8.087  -6.425  -2.646  1.00  0.00
ATOM    585  HB1 PRO  37      -7.650  -5.515  -3.031  1.00  0.00
ATOM    586  HB2 PRO  37      -8.504  -6.999  -3.461  1.00  0.00
ATOM    587  CG  PRO  37      -7.087  -7.224  -1.876  1.00  0.00
ATOM    588  HG1 PRO  37      -6.627  -7.957  -2.522  1.00  0.00
ATOM    589  HG2 PRO  37      -6.338  -6.570  -1.455  1.00  0.00
ATOM    590  CD  PRO  37      -7.857  -7.904  -0.784  1.00  0.00
ATOM    591  HD1 PRO  37      -7.229  -8.071   0.077  1.00  0.00
ATOM    592  HD2 PRO  37      -8.276  -8.834  -1.137  1.00  0.00
ATOM    593  C   PRO  37     -10.569  -6.357  -2.254  1.00  0.00
ATOM    594  O   PRO  37     -11.467  -6.866  -1.584  1.00  0.00
ATOM    595  N   VAL  38     -10.720  -6.015  -3.531  1.00  0.00
ATOM    596  HN  VAL  38      -9.967  -5.610  -4.008  1.00  0.00
ATOM    597  CA  VAL  38     -11.979  -6.221  -4.237  1.00  0.00
ATOM    598  HA  VAL  38     -12.777  -5.842  -3.614  1.00  0.00
ATOM    599  CB  VAL  38     -12.006  -5.450  -5.571  1.00  0.00
ATOM    600  HB  VAL  38     -11.238  -5.856  -6.211  1.00  0.00
ATOM    601  CG1 VAL  38     -11.704  -3.977  -5.342  1.00  0.00
ATOM    602 HG11 VAL  38     -12.002  -3.410  -6.212  1.00  0.00
ATOM    603 HG12 VAL  38     -10.645  -3.848  -5.174  1.00  0.00
ATOM    604 HG13 VAL  38     -12.250  -3.628  -4.479  1.00  0.00
ATOM    605  CG2 VAL  38     -13.347  -5.625  -6.266  1.00  0.00
ATOM    606 HG21 VAL  38     -13.431  -6.636  -6.639  1.00  0.00
ATOM    607 HG22 VAL  38     -13.419  -4.931  -7.090  1.00  0.00
ATOM    608 HG23 VAL  38     -14.145  -5.434  -5.563  1.00  0.00
ATOM    609  C   VAL  38     -12.222  -7.700  -4.511  1.00  0.00
ATOM    610  O   VAL  38     -11.293  -8.508  -4.492  1.00  0.00
ATOM    611  N   LYS  39     -13.477  -8.047  -4.775  1.00  0.00
ATOM    612  HN  LYS  39     -14.173  -7.357  -4.773  1.00  0.00
ATOM    613  CA  LYS  39     -13.850  -9.431  -5.053  1.00  0.00
ATOM    614  HA  LYS  39     -12.960 -10.036  -4.968  1.00  0.00
ATOM    615  CB  LYS  39     -14.898  -9.939  -4.047  1.00  0.00
ATOM    616  HB1 LYS  39     -15.855  -9.996  -4.546  1.00  0.00
ATOM    617  HB2 LYS  39     -14.615 -10.931  -3.727  1.00  0.00
ATOM    618  CG  LYS  39     -15.065  -9.072  -2.804  1.00  0.00
ATOM    619  HG1 LYS  39     -14.989  -8.033  -3.086  1.00  0.00
ATOM    620  HG2 LYS  39     -14.283  -9.315  -2.099  1.00  0.00
ATOM    621  CD  LYS  39     -16.414  -9.301  -2.144  1.00  0.00
ATOM    622  HD1 LYS  39     -17.168  -8.758  -2.693  1.00  0.00
ATOM    623  HD2 LYS  39     -16.640 -10.357  -2.164  1.00  0.00
ATOM    624  CE  LYS  39     -16.415  -8.824  -0.701  1.00  0.00
ATOM    625  HE1 LYS  39     -16.995  -9.516  -0.107  1.00  0.00
ATOM    626  HE2 LYS  39     -15.398  -8.806  -0.340  1.00  0.00
ATOM    627  NZ  LYS  39     -17.002  -7.462  -0.567  1.00  0.00
ATOM    628  HZ1 LYS  39     -17.552  -7.225  -1.417  1.00  0.00
ATOM    629  HZ2 LYS  39     -16.246  -6.758  -0.448  1.00  0.00
ATOM    630  HZ3 LYS  39     -17.630  -7.423   0.261  1.00  0.00
ATOM    631  C   LYS  39     -14.399  -9.563  -6.469  1.00  0.00
ATOM    632  O   LYS  39     -13.886 -10.337  -7.278  1.00  0.00
ATOM    633  N   ARG  40     -15.448  -8.801  -6.759  1.00  0.00
ATOM    634  HN  ARG  40     -15.810  -8.206  -6.070  1.00  0.00
ATOM    635  CA  ARG  40     -16.078  -8.826  -8.074  1.00  0.00
ATOM    636  HA  ARG  40     -15.347  -8.504  -8.800  1.00  0.00
ATOM    637  CB  ARG  40     -16.534 -10.246  -8.417  1.00  0.00
ATOM    638  HB1 ARG  40     -15.676 -10.822  -8.729  1.00  0.00
ATOM    639  HB2 ARG  40     -17.240 -10.197  -9.234  1.00  0.00
ATOM    640  CG  ARG  40     -17.198 -10.968  -7.256  1.00  0.00
ATOM    641  HG1 ARG  40     -18.190 -10.565  -7.115  1.00  0.00
ATOM    642  HG2 ARG  40     -16.612 -10.809  -6.363  1.00  0.00
ATOM    643  CD  ARG  40     -17.305 -12.462  -7.516  1.00  0.00
ATOM    644  HD1 ARG  40     -16.418 -12.788  -8.038  1.00  0.00
ATOM    645  HD2 ARG  40     -18.173 -12.645  -8.133  1.00  0.00
ATOM    646  NE  ARG  40     -17.434 -13.225  -6.277  1.00  0.00
ATOM    647  HE  ARG  40     -17.683 -12.735  -5.466  1.00  0.00
ATOM    648  CZ  ARG  40     -17.235 -14.537  -6.197  1.00  0.00
ATOM    649  NH1 ARG  40     -16.898 -15.225  -7.279  1.00  0.00
ATOM    650 HH11 ARG  40     -16.794 -14.758  -8.157  1.00  0.00
ATOM    651 HH12 ARG  40     -16.748 -16.212  -7.217  1.00  0.00
ATOM    652  NH2 ARG  40     -17.371 -15.160  -5.034  1.00  0.00
ATOM    653 HH21 ARG  40     -17.624 -14.644  -4.216  1.00  0.00
ATOM    654 HH22 ARG  40     -17.220 -16.147  -4.976  1.00  0.00
ATOM    655  C   ARG  40     -17.268  -7.874  -8.116  1.00  0.00
ATOM    656  O   ARG  40     -17.442  -7.122  -9.074  1.00  0.00
ATOM    657  N   THR  41     -18.081  -7.910  -7.065  1.00  0.00
ATOM    658  HN  THR  41     -17.886  -8.530  -6.332  1.00  0.00
ATOM    659  CA  THR  41     -19.252  -7.047  -6.971  1.00  0.00
ATOM    660  HA  THR  41     -19.528  -6.751  -7.973  1.00  0.00
ATOM    661  CB  THR  41     -20.418  -7.806  -6.335  1.00  0.00
ATOM    662  HB  THR  41     -20.623  -8.689  -6.922  1.00  0.00
ATOM    663  OG1 THR  41     -21.586  -7.003  -6.313  1.00  0.00
ATOM    664  HG1 THR  41     -21.499  -6.331  -5.634  1.00  0.00
ATOM    665  CG2 THR  41     -20.139  -8.252  -4.916  1.00  0.00
ATOM    666 HG21 THR  41     -19.793  -7.409  -4.335  1.00  0.00
ATOM    667 HG22 THR  41     -19.281  -9.020  -4.923  1.00  0.00
ATOM    668 HG23 THR  41     -21.065  -8.644  -4.477  1.00  0.00
ATOM    669  C   THR  41     -18.940  -5.797  -6.155  1.00  0.00
ATOM    670  O   THR  41     -19.562  -4.751  -6.338  1.00  0.00
ATOM    671  N   GLU  42     -17.969  -5.915  -5.254  1.00  0.00
ATOM    672  HN  GLU  42     -17.511  -6.776  -5.156  1.00  0.00
ATOM    673  CA  GLU  42     -17.570  -4.797  -4.408  1.00  0.00
ATOM    674  HA  GLU  42     -18.437  -4.480  -3.847  1.00  0.00
ATOM    675  CB  GLU  42     -16.478  -5.238  -3.432  1.00  0.00
ATOM    676  HB1 GLU  42     -15.513  -5.015  -3.864  1.00  0.00
ATOM    677  HB2 GLU  42     -16.556  -6.304  -3.279  1.00  0.00
ATOM    678  CG  GLU  42     -16.561  -4.556  -2.076  1.00  0.00
ATOM    679  HG1 GLU  42     -17.313  -5.054  -1.482  1.00  0.00
ATOM    680  HG2 GLU  42     -16.845  -3.524  -2.224  1.00  0.00
ATOM    681  CD  GLU  42     -15.246  -4.592  -1.323  1.00  0.00
ATOM    682  OE1 GLU  42     -14.293  -3.913  -1.760  1.00  0.00
ATOM    683  OE2 GLU  42     -15.169  -5.300  -0.297  1.00  0.00
ATOM    684  C   GLU  42     -17.072  -3.626  -5.249  1.00  0.00
ATOM    685  O   GLU  42     -17.374  -2.468  -4.959  1.00  0.00
ATOM    686  N   ALA  43     -16.304  -3.935  -6.288  1.00  0.00
ATOM    687  HN  ALA  43     -16.098  -4.877  -6.467  1.00  0.00
ATOM    688  CA  ALA  43     -15.762  -2.908  -7.171  1.00  0.00
ATOM    689  HA  ALA  43     -16.392  -2.035  -7.091  1.00  0.00
ATOM    690  CB  ALA  43     -14.359  -2.518  -6.730  1.00  0.00
ATOM    691  HB1 ALA  43     -14.122  -3.016  -5.801  1.00  0.00
ATOM    692  HB2 ALA  43     -14.310  -1.449  -6.587  1.00  0.00
ATOM    693  HB3 ALA  43     -13.648  -2.813  -7.487  1.00  0.00
ATOM    694  C   ALA  43     -15.753  -3.381  -8.623  1.00  0.00
ATOM    695  O   ALA  43     -14.707  -3.745  -9.159  1.00  0.00
ATOM    696  N   PRO  44     -16.925  -3.378  -9.280  1.00  0.00
ATOM    697  CA  PRO  44     -17.051  -3.815 -10.673  1.00  0.00
ATOM    698  HA  PRO  44     -16.565  -4.754 -10.841  1.00  0.00
ATOM    699  CB  PRO  44     -18.558  -4.006 -10.840  1.00  0.00
ATOM    700  HB1 PRO  44     -18.842  -3.787 -11.859  1.00  0.00
ATOM    701  HB2 PRO  44     -18.824  -5.024 -10.597  1.00  0.00
ATOM    702  CG  PRO  44     -19.165  -3.039  -9.884  1.00  0.00
ATOM    703  HG1 PRO  44     -19.259  -2.070 -10.352  1.00  0.00
ATOM    704  HG2 PRO  44     -20.133  -3.397  -9.564  1.00  0.00
ATOM    705  CD  PRO  44     -18.224  -2.963  -8.711  1.00  0.00
ATOM    706  HD1 PRO  44     -18.173  -1.953  -8.334  1.00  0.00
ATOM    707  HD2 PRO  44     -18.537  -3.642  -7.932  1.00  0.00
ATOM    708  C   PRO  44     -16.532  -2.775 -11.662  1.00  0.00
ATOM    709  O   PRO  44     -16.263  -3.090 -12.821  1.00  0.00
ATOM    710  N   GLY  45     -16.396  -1.536 -11.200  1.00  0.00
ATOM    711  HN  GLY  45     -16.627  -1.340 -10.268  1.00  0.00
ATOM    712  CA  GLY  45     -15.915  -0.473 -12.064  1.00  0.00
ATOM    713  HA1 GLY  45     -15.960  -0.810 -13.089  1.00  0.00
ATOM    714  HA2 GLY  45     -16.560   0.385 -11.950  1.00  0.00
ATOM    715  C   GLY  45     -14.491  -0.059 -11.747  1.00  0.00
ATOM    716  O   GLY  45     -14.134   1.111 -11.883  1.00  0.00
ATOM    717  N   TYR  46     -13.676  -1.020 -11.327  1.00  0.00
ATOM    718  HN  TYR  46     -14.018  -1.934 -11.241  1.00  0.00
ATOM    719  CA  TYR  46     -12.283  -0.748 -10.995  1.00  0.00
ATOM    720  HA  TYR  46     -12.243   0.205 -10.488  1.00  0.00
ATOM    721  CB  TYR  46     -11.739  -1.832 -10.062  1.00  0.00
ATOM    722  HB1 TYR  46     -10.765  -2.142 -10.411  1.00  0.00
ATOM    723  HB2 TYR  46     -12.408  -2.680 -10.078  1.00  0.00
ATOM    724  CG  TYR  46     -11.595  -1.382  -8.625  1.00  0.00
ATOM    725  CD1 TYR  46     -10.623  -1.931  -7.799  1.00  0.00
ATOM    726  HD1 TYR  46      -9.964  -2.690  -8.196  1.00  0.00
ATOM    727  CD2 TYR  46     -12.432  -0.408  -8.095  1.00  0.00
ATOM    728  HD2 TYR  46     -13.194   0.029  -8.724  1.00  0.00
ATOM    729  CE1 TYR  46     -10.487  -1.522  -6.486  1.00  0.00
ATOM    730  HE1 TYR  46      -9.725  -1.960  -5.859  1.00  0.00
ATOM    731  CE2 TYR  46     -12.301   0.007  -6.783  1.00  0.00
ATOM    732  HE2 TYR  46     -12.964   0.766  -6.389  1.00  0.00
ATOM    733  CZ  TYR  46     -11.330  -0.553  -5.983  1.00  0.00
ATOM    734  OH  TYR  46     -11.199  -0.143  -4.676  1.00  0.00
ATOM    735  HH  TYR  46     -10.892  -0.877  -4.139  1.00  0.00
ATOM    736  C   TYR  46     -11.427  -0.671 -12.256  1.00  0.00
ATOM    737  O   TYR  46     -11.940  -0.764 -13.371  1.00  0.00
ATOM    738  N   TYR  47     -10.120  -0.506 -12.072  1.00  0.00
ATOM    739  HN  TYR  47      -9.772  -0.440 -11.159  1.00  0.00
ATOM    740  CA  TYR  47      -9.189  -0.421 -13.195  1.00  0.00
ATOM    741  HA  TYR  47      -8.188  -0.506 -12.800  1.00  0.00
ATOM    742  CB  TYR  47      -9.433  -1.567 -14.181  1.00  0.00
ATOM    743  HB1 TYR  47     -10.224  -1.285 -14.860  1.00  0.00
ATOM    744  HB2 TYR  47      -8.529  -1.748 -14.743  1.00  0.00
ATOM    745  CG  TYR  47      -9.633  -3.862 -13.514  1.00  0.00
ATOM    746  CD1 TYR  47     -10.756  -3.715 -14.105  1.00  0.00
ATOM    747  HD1 TYR  47     -11.188  -3.443 -15.057  1.00  0.00
ATOM    748  CD2 TYR  47      -9.290  -3.229 -12.290  1.00  0.00
ATOM    749  HD2 TYR  47      -8.572  -2.574 -11.818  1.00  0.00
ATOM    750  CE1 TYR  47     -11.124  -4.899 -13.496  1.00  0.00
ATOM    751  HE1 TYR  47     -11.843  -5.550 -13.971  1.00  0.00
ATOM    752  CE2 TYR  47      -9.653  -4.411 -11.674  1.00  0.00
ATOM    753  HE2 TYR  47      -9.219  -4.679 -10.722  1.00  0.00
ATOM    754  CZ  TYR  47     -10.570  -5.242 -12.280  1.00  0.00
ATOM    755  OH  TYR  47     -10.934  -6.421 -11.671  1.00  0.00
ATOM    756  HH  TYR  47     -10.153  -6.958 -11.519  1.00  0.00
ATOM    757  C   TYR  47      -9.318   0.917 -13.916  1.00  0.00
ATOM    758  O   TYR  47      -8.360   1.686 -13.992  1.00  0.00
ATOM    759  N   GLU  48     -10.504   1.184 -14.451  1.00  0.00
ATOM    760  HN  GLU  48     -11.227   0.529 -14.362  1.00  0.00
ATOM    761  CA  GLU  48     -10.754   2.425 -15.175  1.00  0.00
ATOM    762  HA  GLU  48     -10.103   2.441 -16.037  1.00  0.00
ATOM    763  CB  GLU  48     -12.209   2.478 -15.648  1.00  0.00
ATOM    764  HB1 GLU  48     -12.454   3.529 -14.784  1.00  0.00
ATOM    765  HB2 GLU  48     -12.349   3.368 -16.244  1.00  0.00
ATOM    766  CG  GLU  48     -12.621   1.276 -16.482  1.00  0.00
ATOM    767  HG1 GLU  48     -12.135   1.337 -17.444  1.00  0.00
ATOM    768  HG2 GLU  48     -12.304   0.376 -15.976  1.00  0.00
ATOM    769  CD  GLU  48     -14.120   1.204 -16.702  1.00  0.00
ATOM    770  OE1 GLU  48     -14.858   1.919 -15.994  1.00  0.00
ATOM    771  OE2 GLU  48     -14.554   0.433 -17.584  1.00  0.00
ATOM    772  C   GLU  48     -10.445   3.639 -14.306  1.00  0.00
ATOM    773  O   GLU  48     -10.136   4.716 -14.815  1.00  0.00
ATOM    774  N   VAL  49     -10.529   3.459 -12.992  1.00  0.00
ATOM    775  HN  VAL  49     -10.761   2.578 -12.644  1.00  0.00
ATOM    776  CA  VAL  49     -10.261   4.545 -12.055  1.00  0.00
ATOM    777  HA  VAL  49      -9.905   5.392 -12.624  1.00  0.00
ATOM    778  CB  VAL  49     -11.542   4.971 -11.313  1.00  0.00
ATOM    779  HB  VAL  49     -12.308   5.171 -12.047  1.00  0.00
ATOM    780  CG1 VAL  49     -12.033   3.853 -10.407  1.00  0.00
ATOM    781 HG11 VAL  49     -11.630   3.991  -9.414  1.00  0.00
ATOM    782 HG12 VAL  49     -11.705   2.901 -10.799  1.00  0.00
ATOM    783 HG13 VAL  49     -13.112   3.872 -10.364  1.00  0.00
ATOM    784  CG2 VAL  49     -11.301   6.246 -10.518  1.00  0.00
ATOM    785 HG21 VAL  49     -10.706   6.020  -9.646  1.00  0.00
ATOM    786 HG22 VAL  49     -12.249   6.461 -10.209  1.00  0.00
ATOM    787 HG23 VAL  49     -10.779   6.963 -11.135  1.00  0.00
ATOM    788  C   VAL  49      -9.195   4.160 -11.026  1.00  0.00
ATOM    789  O   VAL  49      -8.861   4.956 -10.148  1.00  0.00
ATOM    790  N   ILE  50      -8.665   2.941 -11.130  1.00  0.00
ATOM    791  HN  ILE  50      -8.958   2.147 -11.647  1.00  0.00
ATOM    792  CA  ILE  50      -7.644   2.474 -10.204  1.00  0.00
ATOM    793  HA  ILE  50      -7.342   3.309  -9.589  1.00  0.00
ATOM    794  CB  ILE  50      -8.182   1.365  -9.282  1.00  0.00
ATOM    795  HB  ILE  50      -8.267   0.458  -9.861  1.00  0.00
ATOM    796  CG1 ILE  50      -9.559   1.747  -8.737  1.00  0.00
ATOM    797 HG11 ILE  50     -10.222   1.952  -9.564  1.00  0.00
ATOM    798 HG12 ILE  50      -9.952   0.921  -8.162  1.00  0.00
ATOM    799  CG2 ILE  50      -7.210   1.105  -8.142  1.00  0.00
ATOM    800 HG21 ILE  50      -6.248   1.528  -8.387  1.00  0.00
ATOM    801 HG22 ILE  50      -7.108   0.041  -7.991  1.00  0.00
ATOM    802 HG23 ILE  50      -7.586   1.561  -7.238  1.00  0.00
ATOM    803  CD1 ILE  50      -9.540   2.967  -7.843  1.00  0.00
ATOM    804 HD11 ILE  50      -9.670   3.855  -8.443  1.00  0.00
ATOM    805 HD12 ILE  50      -8.593   3.019  -7.325  1.00  0.00
ATOM    806 HD13 ILE  50     -10.341   2.898  -7.123  1.00  0.00
ATOM    807  C   ILE  50      -6.428   1.945 -10.953  1.00  0.00
ATOM    808  O   ILE  50      -6.557   1.228 -11.948  1.00  0.00
ATOM    809  N   ARG  51      -5.248   2.301 -10.486  1.00  0.00
ATOM    810  HN  ARG  51      -5.216   2.877  -9.676  1.00  0.00
ATOM    811  CA  ARG  51      -4.000   1.873 -11.085  1.00  0.00
ATOM    812  HA  ARG  51      -4.014   2.198 -12.114  1.00  0.00
ATOM    813  CB  ARG  51      -2.811   2.519 -10.373  1.00  0.00
ATOM    814  HB1 ARG  51      -3.181   3.123  -9.557  1.00  0.00
ATOM    815  HB2 ARG  51      -2.177   1.740  -9.975  1.00  0.00
ATOM    816  CG  ARG  51      -1.967   3.403 -11.277  1.00  0.00
ATOM    817  HG1 ARG  51      -2.041   3.037 -12.291  1.00  0.00
ATOM    818  HG2 ARG  51      -0.939   3.358 -10.950  1.00  0.00
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ATOM    819  CD  ARG  51      -2.433   4.849 -11.240  1.00  0.00
ATOM    820  NE1 ARG  51      -2.996   5.010 -10.332  1.00  0.00
ATOM    821  HD2 ARG  51      -1.566   5.493 -11.244  1.00  0.00
ATOM    822  NE  ARG  51      -3.275   5.184 -12.765  1.00  0.00
ATOM    823  HE  ARG  51      -4.217   5.390 -12.212  1.00  0.00
ATOM    824  CZ  ARG  51      -2.832   5.226 -13.638  1.00  0.00
ATOM    825  NH1 ARG  51      -1.562   4.953 -13.904  1.00  0.00
ATOM    826  HH11 ARG  51      -1.231   4.984 -14.846  1.00  0.00
ATOM    827  HH12 ARG  51      -0.936   4.716 -13.161  1.00  0.00
ATOM    828  NH2 ARG  51      -3.659   5.539 -14.626  1.00  0.00
ATOM    829  HH21 ARG  51      -3.323   5.569 -15.568  1.00  0.00
ATOM    830  HH22 ARG  51      -4.617   5.746 -14.430  1.00  0.00
ATOM    831  C   ARG  51      -3.864   0.354 -11.056  1.00  0.00
ATOM    832  O   ARG  51      -4.094  -0.319 -12.061  1.00  0.00
ATOM    833  N   SER  52      -3.479  -0.182  -9.901  1.00  0.00
ATOM    834  HN  SER  52      -3.310   0.403  -9.134  1.00  0.00
ATOM    835  CA  SER  52      -3.307  -1.622  -9.751  1.00  0.00
ATOM    836  HA  SER  52      -3.766  -2.101 -10.603  1.00  0.00
ATOM    837  CB  SER  52      -1.820  -1.980  -9.715  1.00  0.00
ATOM    838  HB1 SER  52      -1.690  -3.005 -10.027  1.00  0.00
ATOM    839  HB2 SER  52      -1.447  -1.860  -8.708  1.00  0.00
ATOM    840  OG  SER  52      -1.072  -1.143 -10.580  1.00  0.00
ATOM    841  HG  SER  52      -0.287  -1.608 -10.877  1.00  0.00
ATOM    842  C   SER  52      -3.993  -2.128  -8.488  1.00  0.00
ATOM    843  O   SER  52      -3.353  -2.308  -7.452  1.00  0.00
ATOM    844  N   PRO  53      -5.310  -2.379  -8.565  1.00  0.00
ATOM    845  CA  PRO  53      -6.087  -2.882  -7.435  1.00  0.00
ATOM    846  HA  PRO  53      -6.390  -2.083  -6.773  1.00  0.00
ATOM    847  CB  PRO  53      -7.313  -3.484  -8.111  1.00  0.00
ATOM    848  HB1 PRO  53      -8.160  -3.415  -7.450  1.00  0.00
ATOM    849  HB2 PRO  53      -7.122  -4.519  -8.355  1.00  0.00
ATOM    850  CG  PRO  53      -7.512  -2.661  -9.337  1.00  0.00
ATOM    851  HG1 PRO  53      -7.963  -3.263 -10.110  1.00  0.00
ATOM    852  HG2 PRO  53      -8.139  -1.812  -9.109  1.00  0.00
ATOM    853  CD  PRO  53      -6.145  -2.197  -9.770  1.00  0.00
ATOM    854  HD1 PRO  53      -5.780  -2.805 -10.584  1.00  0.00
ATOM    855  HD2 PRO  53      -6.176  -1.157 -10.060  1.00  0.00
ATOM    856  C   PRO  53      -5.340  -3.947  -6.639  1.00  0.00
ATOM    857  O   PRO  53      -5.425  -5.137  -6.943  1.00  0.00
ATOM    858  N   MET  54      -4.609  -3.512  -5.619  1.00  0.00
ATOM    859  HN  MET  54      -4.581  -2.552  -5.426  1.00  0.00
ATOM    860  CA  MET  54      -3.850  -4.428  -4.777  1.00  0.00
ATOM    861  HA  MET  54      -4.300  -5.405  -4.859  1.00  0.00
ATOM    862  CB  MET  54      -2.398  -4.508  -5.251  1.00  0.00
ATOM    863  HB1 MET  54      -2.390  -4.624  -6.327  1.00  0.00
ATOM    864  HB2 MET  54      -1.897  -3.587  -4.995  1.00  0.00
ATOM    865  CG  MET  54      -1.615  -5.660  -4.644  1.00  0.00
ATOM    866  HG1 MET  54      -1.472  -5.664  -3.592  1.00  0.00
ATOM    867  HG2 MET  54      -0.653  -5.720  -5.132  1.00  0.00
ATOM    868  SD  MET  54      -2.452  -7.247  -4.826  1.00  0.00
ATOM    869  CE  MET  54      -3.383  -7.311  -3.298  1.00  0.00
ATOM    870  HE1 MET  54      -2.905  -7.997  -2.612  1.00  0.00
ATOM    871  HE2 MET  54      -4.388  -7.650  -3.501  1.00  0.00
ATOM    872  HE3 MET  54      -3.418  -6.327  -2.857  1.00  0.00
ATOM    873  C   MET  54      -3.897  -3.984  -3.320  1.00  0.00
ATOM    874  O   MET  54      -2.937  -3.415  -2.802  1.00  0.00
ATOM    875  N   ASP  55      -5.026  -4.240  -2.667  1.00  0.00
ATOM    876  HN  ASP  55      -5.755  -4.699  -3.134  1.00  0.00
ATOM    877  CA  ASP  55      -5.201  -3.870  -1.269  1.00  0.00
ATOM    878  HA  ASP  55      -4.803  -2.874  -1.139  1.00  0.00
ATOM    879  CB  ASP  55      -6.690  -3.863  -0.906  1.00  0.00
ATOM    880  HB1 ASP  55      -6.811  -3.495   0.102  1.00  0.00
ATOM    881  HB2 ASP  55      -7.075  -4.869  -0.964  1.00  0.00
ATOM    882  CG  ASP  55      -7.506  -2.985  -1.835  1.00  0.00
ATOM    883  OD1 ASP  55      -7.575  -3.302  -3.041  1.00  0.00
ATOM    884  OD2 ASP  55      -8.074  -1.961  -1.357  1.00  0.00
ATOM    885  C   ASP  55      -4.435  -4.826  -0.360  1.00  0.00
ATOM    886  O   ASP  55      -3.578  -5.580  -0.819  1.00  0.00
ATOM    887  N   LEU  56      -4.739  -4.786   0.931  1.00  0.00
ATOM    888  HN  LEU  56      -5.426  -4.163   1.242  1.00  0.00
ATOM    889  CA  LEU  56      -4.069  -5.644   1.898  1.00  0.00
ATOM    890  HA  LEU  56      -3.012  -5.620   1.683  1.00  0.00
ATOM    891  CB  LEU  56      -4.305  -5.115   3.318  1.00  0.00
ATOM    892  HB1 LEU  56      -4.223  -5.939   4.008  1.00  0.00
ATOM    893  HB2 LEU  56      -5.306  -4.729   3.371  1.00  0.00
ATOM    894  CG  LEU  56      -3.343  -4.015   3.770  1.00  0.00
ATOM    895  HG  LEU  56      -3.605  -3.702   4.770  1.00  0.00
ATOM    896  CD1 LEU  56      -3.425  -2.802   2.859  1.00  0.00
ATOM    897  HD11 LEU  56      -3.644  -1.924   3.449  1.00  0.00
ATOM    898  HD12 LEU  56      -4.204  -2.950   2.132  1.00  0.00
ATOM    899  HD13 LEU  56      -2.481  -2.668   2.352  1.00  0.00
ATOM    900  CD2 LEU  56      -1.929  -4.544   3.801  1.00  0.00
ATOM    901  HD21 LEU  56      -1.279  -3.850   3.291  1.00  0.00
ATOM    902  HD22 LEU  56      -1.898  -5.500   3.303  1.00  0.00
ATOM    903  HD23 LEU  56      -1.611  -4.656   4.824  1.00  0.00
ATOM    904  C   LEU  56      -4.568  -7.081   1.773  1.00  0.00
ATOM    905  O   LEU  56      -5.294  -7.404   0.835  1.00  0.00
ATOM    906  N   LYS  57      -4.152  -7.939   2.706  1.00  0.00
ATOM    907  HN  LYS  57      -3.564  -7.617   3.417  1.00  0.00
ATOM    908  CA  LYS  57      -4.556  -9.347   2.715  1.00  0.00
ATOM    909  HA  LYS  57      -4.259  -9.758   3.669  1.00  0.00
ATOM    910  CB  LYS  57      -4.075  -9.490   2.576  1.00  0.00
ATOM    911  HB1 LYS  57      -4.349  -9.007   3.418  1.00  0.00
ATOM    912  HB2 LYS  57      -6.396  -9.008   1.668  1.00  0.00
ATOM    913  CG  LYS  57      -6.542 -10.935   2.530  1.00  0.00
ATOM    914  HG1 LYS  57      -6.160 -11.395   1.629  1.00  0.00
ATOM    915  HG2 LYS  57      -7.622 -10.954   2.517  1.00  0.00
ATOM    916  CD  LYS  57      -6.049 -11.720   3.736  1.00  0.00
ATOM    917  HD1 LYS  57      -5.946 -11.047   4.573  1.00  0.00
ATOM    918  HD2 LYS  57      -5.090 -12.157   3.498  1.00  0.00
ATOM    919  CE  LYS  57      -7.017 -12.831   4.112  1.00  0.00
ATOM    920  HE1 LYS  57      -7.967 -12.640   3.635  1.00  0.00
ATOM    921  HE2 LYS  57      -6.621 -13.771   3.759  1.00  0.00
ATOM    922  NZ  LYS  57      -7.223 -12.915   5.585  1.00  0.00
ATOM    923  HZ1 LYS  57      -6.363 -12.609   6.084  1.00  0.00
ATOM    924  HZ2 LYS  57      -7.441 -13.894   5.860  1.00  0.00
ATOM    925  HZ3 LYS  57      -8.013 -12.302   5.871  1.00  0.00
ATOM    926  C   LYS  57      -3.855 -10.144   1.617  1.00  0.00
ATOM    927  O   LYS  57      -3.197 -11.146   1.895  1.00  0.00
ATOM    928  N   THR  58      -4.014  -9.714   0.370  1.00  0.00
ATOM    929  HN  THR  58      -4.551  -8.913   0.201  1.00  0.00
ATOM    930  CA  THR  58      -3.403 -10.411  -0.755  1.00  0.00
ATOM    931  HA  THR  58      -3.409 -11.465  -0.527  1.00  0.00
ATOM    932  CB  THR  58      -4.223 -10.177  -2.031  1.00  0.00
ATOM    933  HB  THR  58      -4.448  -9.126  -2.112  1.00  0.00
ATOM    934  OG1 THR  58      -5.448 -10.887  -1.970  1.00  0.00
ATOM    935  HG1 THR  58      -5.974 -10.567  -1.238  1.00  0.00
ATOM    936  CG2 THR  58      -3.515 -10.898  -3.304  1.00  0.00
ATOM    937  HG21 THR  58      -4.236 -11.003  -3.999  1.00  0.00
ATOM    938  HG22 THR  58      -2.775 -11.349  -3.073  1.00  0.00
ATOM    939  HG23 THR  58      -3.031  -9.740  -3.747  1.00  0.00
ATOM    940  C   THR  58      -1.956  -9.961  -0.952  1.00  0.00
ATOM    941  O   THR  58      -1.093 -10.759  -1.318  1.00  0.00
ATOM    942  N   MET  59      -1.697  -8.682  -0.701  1.00  0.00
ATOM    943  HN  MET  59      -2.424  -8.092  -0.413  1.00  0.00
ATOM    944  CA  MET  59      -0.355  -8.132  -0.851  1.00  0.00
ATOM    945  HA  MET  59       0.020  -8.431  -1.819  1.00  0.00
ATOM    946  CB  MET  59      -0.404  -6.605  -0.783  1.00  0.00
ATOM    947  HB1 MET  59       0.536  -6.209  -1.138  1.00  0.00
ATOM    948  HB2 MET  59      -1.200  -6.252  -1.421  1.00  0.00
ATOM    949  CG  MET  59      -0.650  -6.072   0.617  1.00  0.00
ATOM    950  HG1 MET  59      -1.503  -6.586   1.032  1.00  0.00
ATOM    951  HG2 MET  59       0.218  -6.279   1.223  1.00  0.00
ATOM    952  SD  MET  59      -0.969  -4.297   0.643  1.00  0.00
ATOM    953  CE  MET  59       0.230  -3.715  -0.554  1.00  0.00
ATOM    954  HE1 MET  59       0.178  -4.324  -1.443  1.00  0.00
ATOM    955  HE2 MET  59       1.221  -3.779  -0.131  1.00  0.00
ATOM    956  HE3 MET  59       0.016  -2.688  -0.808  1.00  0.00
ATOM    957  C   MET  59       0.582  -8.669   0.228  1.00  0.00
ATOM    958  O   MET  59       1.701  -9.092  -0.061  1.00  0.00
ATOM    959  N   SER  60       0.126  -8.621   1.476  1.00  0.00
ATOM    960  HN  SER  60      -0.772  -8.270   1.644  1.00  0.00
ATOM    961  CA  SER  60       0.925  -9.088   2.601  1.00  0.00
ATOM    962  HA  SER  60       1.769  -8.445   2.682  1.00  0.00
ATOM    963  CB  SER  60       0.117  -9.004   3.898  1.00  0.00
ATOM    964  HB1 SER  60       0.214  -8.013   4.315  1.00  0.00
ATOM    965  HB2 SER  60      -0.922  -9.205   3.686  1.00  0.00
ATOM    966  OG  SER  60       0.579  -9.946   4.652  1.00  0.00
ATOM    967  HG  SER  60       1.273  -9.548   5.383  1.00  0.00
ATOM    968  C   SER  60       1.401 -10.517   2.372  1.00  0.00
ATOM    969  O   SER  60       2.417 -10.939   2.923  1.00  0.00
ATOM    970  N   GLU  61       0.665 -11.258   1.551  1.00  0.00
ATOM    971  HN  GLU  61      -0.134 -10.867   1.137  1.00  0.00
ATOM    972  CA  GLU  61       1.022 -12.636   1.249  1.00  0.00
ATOM    973  HA  GLU  61       1.138 -13.156   2.186  1.00  0.00
ATOM    974  CB  GLU  61      -0.086 -13.309   0.435  1.00  0.00
ATOM    975  HB1 GLU  61       0.025 -14.380   0.516  1.00  0.00
ATOM    976  HB2 GLU  61       0.021 -13.022  -0.601  1.00  0.00
ATOM    977  CG  GLU  61      -1.484 -12.937   0.891  1.00  0.00
ATOM    978  HG1 GLU  61      -1.460 -12.730   1.951  1.00  0.00
ATOM    979  HG2 GLU  61      -1.797 -12.051   0.360  1.00  0.00
ATOM    980  CD  GLU  61      -2.493 -14.039   0.636  1.00  0.00
ATOM    981  OE1 GLU  61      -2.755 -14.830   1.567  1.00  0.00
ATOM    982  OE2 GLU  61      -3.020 -14.112  -0.494  1.00  0.00
ATOM    983  C   GLU  61       2.338 -12.695   0.485  1.00  0.00
ATOM    984  O   GLU  61       3.295 -13.334   0.922  1.00  0.00
ATOM    985  N   ARG  62       2.382 -12.013  -0.654  1.00  0.00
ATOM    986  HN  ARG  62       1.588 -11.524  -0.949  1.00  0.00
ATOM    987  CA  ARG  62       3.578 -11.980  -1.479  1.00  0.00
ATOM    988  HA  ARG  62       3.752 -12.979  -1.846  1.00  0.00
ATOM    989  CB  ARG  62       3.368 -11.045  -2.672  1.00  0.00
ATOM    990  HB1 ARG  62       4.330 -10.804  -3.101  1.00  0.00
ATOM    991  HB2 ARG  62       2.898 -10.136  -2.326  1.00  0.00
ATOM    992  CG  ARG  62       2.496 -11.652  -3.761  1.00  0.00
ATOM    993  HG1 ARG  62       1.895 -12.438  -3.328  1.00  0.00
ATOM    994  HG2 ARG  62       3.131 -12.065  -4.528  1.00  0.00
ATOM    995  CD  ARG  62       1.576 -10.619  -4.389  1.00  0.00
ATOM    996  HD1 ARG  62       2.043  -9.647  -4.320  1.00  0.00
ATOM    997  HD2 ARG  62       0.645 -10.609  -3.845  1.00  0.00
ATOM    998  NE  ARG  62       1.299 -10.916  -5.792  1.00  0.00
ATOM    999  HE  ARG  62       1.697 -10.330  -6.467  1.00  0.00
ATOM   1000  CZ  ARG  62       0.541 -11.931  -6.194  1.00  0.00
ATOM   1001  NH1 ARG  62       0.336 -12.136  -7.488  1.00  0.00
ATOM   1002  HH11 ARG  62       0.753 -11.527  -8.163  1.00  0.00
ATOM   1003  HH12 ARG  62      -0.235 -12.900  -7.789  1.00  0.00
ATOM   1004  NH2 ARG  62      -0.014 -12.742  -5.303  1.00  0.00
ATOM   1005  HH21 ARG  62       0.139 -12.590  -4.326  1.00  0.00
ATOM   1006  HH22 ARG  62      -0.583 -13.505  -5.608  1.00  0.00
ATOM   1007  C   ARG  62       4.790 -11.542  -0.664  1.00  0.00
ATOM   1008  O   ARG  62       5.781 -12.266  -0.576  1.00  0.00
ATOM   1009  N   LEU  63       4.700 -10.366  -0.052  1.00  0.00
ATOM   1010  HN  LEU  63       3.882  -9.835  -0.149  1.00  0.00
ATOM   1011  CA  LEU  63       5.792  -9.853   0.768  1.00  0.00
ATOM   1012  HA  LEU  63       6.634  -9.663   0.117  1.00  0.00
ATOM   1013  CB  LEU  63       5.384  -8.546   1.450  1.00  0.00
ATOM   1014  HB1 LEU  63       5.208  -7.805   0.685  1.00  0.00
ATOM   1015  HB2 LEU  63       4.460  -8.716   1.982  1.00  0.00
ATOM   1016  CG  LEU  63       6.413  -7.984   2.436  1.00  0.00
ATOM   1017  HG  LEU  63       7.141  -8.747   2.663  1.00  0.00
ATOM   1018  CD1 LEU  63       7.148  -6.804   1.825  1.00  0.00
ATOM   1019  HD11 LEU  63       6.457  -5.991   1.672  1.00  0.00
ATOM   1020  HD12 LEU  63       7.575  -7.097   0.877  1.00  0.00
ATOM   1021  HD13 LEU  63       7.937  -6.467   2.492  1.00  0.00
ATOM   1022  CD2 LEU  63       5.741  -9.580   3.738  1.00  0.00
ATOM   1023  HD21 LEU  63       4.709  -7.899   3.726  1.00  0.00
ATOM   1024  HD22 LEU  63       5.785  -6.507   3.848  1.00  0.00
ATOM   1025  HD23 LEU  63       6.252  -8.049   4.565  1.00  0.00
ATOM   1026  C   LEU  63       6.204 -10.880   1.817  1.00  0.00
ATOM   1027  O   LEU  63       7.391 -11.134   2.019  1.00  0.00
ATOM   1028  N   LYS  64       5.212 -11.476   2.475  1.00  0.00
ATOM   1029  HN  LYS  64       4.267 -11.235   2.262  1.00  0.00
ATOM   1030  CA  LYS  64       5.469 -12.487   3.493  1.00  0.00
ATOM   1031  HA  LYS  64       5.942 -12.002   4.333  1.00  0.00
ATOM   1032  CB  LYS  64       4.155 -13.122   3.953  1.00  0.00
ATOM   1033  HB1 LYS  64       3.506 -13.240   3.098  1.00  0.00
ATOM   1034  HB2 LYS  64       4.365 -14.094   4.372  1.00  0.00
ATOM   1035  CG  LYS  64       3.416 -12.301   5.000  1.00  0.00
ATOM   1036  HG1 LYS  64       3.615 -11.254   4.826  1.00  0.00
ATOM   1037  HG2 LYS  64       2.396 -12.488   4.907  1.00  0.00
ATOM   1038  CD  LYS  64       3.859 -12.662   6.408  1.00  0.00
ATOM   1039  HD1 LYS  64       3.007 -13.038   6.957  1.00  0.00
ATOM   1040  HD2 LYS  64       4.618 -13.428   6.351  1.00  0.00
ATOM   1041  CE  LYS  64       4.424 -11.459   7.141  1.00  0.00
ATOM   1042  HE1 LYS  64       4.711 -10.712   6.414  1.00  0.00
ATOM   1043  HE2 LYS  64       3.663 -11.056   7.790  1.00  0.00
ATOM   1044  NZ  LYS  64       5.618 -11.817   7.959  1.00  0.00
ATOM   1045  HZ1 LYS  64       6.086 -12.655   7.560  1.00  0.00
ATOM   1046  HZ2 LYS  64       5.332 -12.025   8.936  1.00  0.00
ATOM   1047  HZ3 LYS  64       6.295 -11.028   7.968  1.00  0.00
ATOM   1048  C   LYS  64       6.407 -13.562   2.953  1.00  0.00
ATOM   1049  O   LYS  64       7.255 -14.082   3.677  1.00  0.00
ATOM   1050  N   ASN  65       6.256 -13.879   1.671  1.00  0.00
ATOM   1051  HN  ASN  65       5.569 -13.420   1.143  1.00  0.00
ATOM   1052  CA  ASN  65       7.103 -14.872   1.023  1.00  0.00
ATOM   1053  HA  ASN  65       7.632 -15.410   1.795  1.00  0.00
ATOM   1054  CB  ASN  65       6.254 -15.855   0.214  1.00  0.00
ATOM   1055  HB1 ASN  65       6.762 -16.082  -0.712  1.00  0.00
ATOM   1056  HB2 ASN  65       5.299 -15.400  -0.006  1.00  0.00
ATOM   1057  CG  ASN  65       6.006 -17.155   0.954  1.00  0.00
ATOM   1058  OD1 ASN  65       6.266 -18.239   0.433  1.00  0.00
ATOM   1059  ND2 ASN  65       5.501 -17.052   2.178  1.00  0.00
ATOM   1060  HD21 ASN  65       5.318 -16.156   2.530  1.00  0.00
ATOM   1061  HD22 ASN  65       5.331 -17.877   2.679  1.00  0.00
ATOM   1062  C   ASN  65       8.122 -14.195   0.119  1.00  0.00
ATOM   1063  O   ASN  65       8.532 -14.749  -0.901  1.00  0.00
ATOM   1064  N   ARG  66       8.535 -12.995   0.510  1.00  0.00
ATOM   1065  HN  ARG  66       8.174 -12.614   1.338  1.00  0.00
ATOM   1066  CA  ARG  66       9.524 -12.235  -0.247  1.00  0.00
ATOM   1067  HA  ARG  66       9.535 -11.232   0.148  1.00  0.00
ATOM   1068  CB  ARG  66      10.919 -12.848  -0.092  1.00  0.00
ATOM   1069  HB1 ARG  66      11.122 -13.471  -0.950  1.00  0.00
ATOM   1070  HB2 ARG  66      11.643 -12.051  -0.063  1.00  0.00
ATOM   1071  CG  ARG  66      11.100 -13.692   1.161  1.00  0.00
ATOM   1072  HG1 ARG  66      11.963 -14.321   1.031  1.00  0.00
ATOM   1073  HG2 ARG  66      10.225 -14.307   1.303  1.00  0.00
ATOM   1074  CD  ARG  66      11.298 -12.825   2.392  1.00  0.00
ATOM   1075  HD1 ARG  66      11.969 -12.017   2.143  1.00  0.00
ATOM   1076  HD2 ARG  66      10.342 -12.420   2.689  1.00  0.00
ATOM   1077  NE  ARG  66      11.860 -13.560   3.509  1.00  0.00
ATOM   1078  HE  ARG  66      12.826 -13.512   3.663  1.00  0.00
ATOM   1079  CZ  ARG  66      11.136 -14.344   4.319  1.00  0.00
ATOM   1080  NH1 ARG  66      11.719 -14.996   5.314  1.00  0.00
ATOM   1081  HH11 ARG  66      12.706 -14.917   5.455  1.00  0.00
ATOM   1082  HH12 ARG  66      11.173 -15.573   5.921  1.00  0.00
ATOM   1083  NH2 ARG  66       9.827 -14.454   4.136  1.00  0.00
ATOM   1084  HH21 ARG  66       9.384 -13.963   3.387  1.00  0.00
ATOM   1085  HH22 ARG  66       9.284 -15.030   4.747  1.00  0.00
ATOM   1086  C   ARG  66       9.152 -12.177  -1.725  1.00  0.00
ATOM   1087  O   ARG  66      10.018 -12.041  -2.590  1.00  0.00
ATOM   1088  N   TYR  67       7.862 -12.285  -2.002  1.00  0.00
ATOM   1089  HN  TYR  67       7.230 -12.408  -1.266  1.00  0.00
ATOM   1090  CA  TYR  67       7.364 -12.275  -3.374  1.00  0.00
ATOM   1091  HA  TYR  67       8.125 -12.708  -4.006  1.00  0.00
ATOM   1092  CB  TYR  67       6.091 -13.117  -3.475  1.00  0.00
ATOM   1093  HB1 TYR  67       6.193 -13.995  -2.856  1.00  0.00
ATOM   1094  HB2 TYR  67       5.259 -12.530  -3.121  1.00  0.00
ATOM   1095  CG  TYR  67       5.767 -13.566  -4.881  1.00  0.00
ATOM   1096  CD1 TYR  67       6.113 -14.835  -5.326  1.00  0.00
ATOM   1097  HD1 TYR  67       6.628 -15.506  -4.654  1.00  0.00
ATOM   1098  CD2 TYR  67       5.107 -13.720  -5.761  1.00  0.00
ATOM   1099  HD2 TYR  67       4.827 -11.731  -5.427  1.00  0.00
ATOM   1100  CE1 TYR  67       5.811 -15.247  -6.611  1.00  0.00
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ATOM   1101  HE1 TYR    67       6.089 -16.237  -6.940  1.00  0.00
ATOM   1102  CE2 TYR    67       4.798 -13.123  -7.044  1.00  0.00
ATOM   1103  HE2 TYR    67       4.281 -12.449  -7.711  1.00  0.00
ATOM   1104  CZ  TYR    67       5.153 -14.387  -7.466  1.00  0.00
ATOM   1105  OH  TYR    67       4.850 -14.791  -8.745  1.00  0.00
ATOM   1106  HH  TYR    67       4.026 -15.286  -8.737  1.00  0.00
ATOM   1107  C   TYR    67       7.066 -10.860  -3.859  1.00  0.00
ATOM   1108  O   TYR    67       6.990 -10.616  -5.063  1.00  0.00
ATOM   1109  N   TYR    68       6.859  -9.937  -2.925  1.00  0.00
ATOM   1110  HN  TYR    68       6.909 -10.187  -1.978  1.00  0.00
ATOM   1111  CA  TYR    68       6.515  -8.568  -3.280  1.00  0.00
ATOM   1112  HA  TYR    68       6.570  -8.478  -4.355  1.00  0.00
ATOM   1113  CB  TYR    68       5.089  -8.263  -2.821  1.00  0.00
ATOM   1114  HB1 TYR    68       4.746  -9.065  -2.186  1.00  0.00
ATOM   1115  HB2 TYR    68       5.096  -7.348  -2.256  1.00  0.00
ATOM   1116  CG  TYR    68       4.089  -8.103  -3.946  1.00  0.00
ATOM   1117  CD1 TYR    68       4.278  -8.729  -5.174  1.00  0.00
ATOM   1118  HD1 TYR    68       5.157  -9.336  -5.327  1.00  0.00
ATOM   1119  CD2 TYR    68       2.946  -7.334  -3.772  1.00  0.00
ATOM   1120  HD2 TYR    68       2.783  -6.844  -2.823  1.00  0.00
ATOM   1121  CE1 TYR    68       3.359  -8.582  -6.196  1.00  0.00
ATOM   1122  HE1 TYR    68       3.523  -9.075  -7.143  1.00  0.00
ATOM   1123  CE2 TYR    68       2.022  -7.185  -4.789  1.00  0.00
ATOM   1124  HE2 TYR    68       1.141  -6.581  -4.633  1.00  0.00
ATOM   1125  CZ  TYR    68       2.233  -7.811  -5.998  1.00  0.00
ATOM   1126  OH  TYR    68       1.315  -7.665  -7.012  1.00  0.00
ATOM   1127  HH  TYR    68       0.444  -7.518  -6.637  1.00  0.00
ATOM   1128  C   TYR    68       7.484  -7.570  -2.656  1.00  0.00
ATOM   1129  O   TYR    68       7.096  -6.457  -2.303  1.00  0.00
ATOM   1130  N   VAL    69       8.744  -7.967  -2.529  1.00  0.00
ATOM   1131  HN  VAL    69       9.000  -8.862  -2.835  1.00  0.00
ATOM   1132  CA  VAL    69       9.761  -7.086  -1.962  1.00  0.00
ATOM   1133  HA  VAL    69       9.284  -6.461  -1.221  1.00  0.00
ATOM   1134  CB  VAL    69      10.907  -7.854  -1.276  1.00  0.00
ATOM   1135  HB  VAL    69      11.715  -7.964  -1.984  1.00  0.00
ATOM   1136  CG1 VAL    69      10.465  -9.242  -0.846  1.00  0.00
ATOM   1137  HG11 VAL    69       9.487  -9.183  -0.393  1.00  0.00
ATOM   1138  HG12 VAL    69      11.171  -9.640  -0.133  1.00  0.00
ATOM   1139  HG13 VAL    69      10.423  -9.887  -1.712  1.00  0.00
ATOM   1140  CG2 VAL    69      11.423  -7.059  -0.090  1.00  0.00
ATOM   1141  HG21 VAL    69      12.197  -7.619   0.411  1.00  0.00
ATOM   1142  HG22 VAL    69      10.608  -6.872   0.597  1.00  0.00
ATOM   1143  HG23 VAL    69      11.822  -6.118  -0.438  1.00  0.00
ATOM   1144  C   VAL    69      10.352  -6.189  -3.043  1.00  0.00
ATOM   1145  O   VAL    69      11.543  -6.272  -3.345  1.00  0.00
ATOM   1146  N   SER    70       9.507  -5.372  -3.634  1.00  0.00
ATOM   1147  HN  SER    70       8.566  -5.371  -3.359  1.00  0.00
ATOM   1148  CA  SER    70       9.934  -4.491  -4.703  1.00  0.00
ATOM   1149  HA  SER    70      10.985  -4.285  -4.564  1.00  0.00
ATOM   1150  CB  SER    70       9.734  -5.190  -6.045  1.00  0.00
ATOM   1151  HB1 SER    70      10.626  -5.749  -6.289  1.00  0.00
ATOM   1152  HB2 SER    70       8.898  -5.868  -5.966  1.00  0.00
ATOM   1153  OG  SER    70       9.476  -4.258  -7.081  1.00  0.00
ATOM   1154  HG  SER    70      10.175  -3.600  -7.102  1.00  0.00
ATOM   1155  C   SER    70       9.164  -3.179  -4.657  1.00  0.00
ATOM   1156  O   SER    70       7.969  -3.158  -4.359  1.00  0.00
ATOM   1157  N   LYS    71       9.861  -2.083  -4.924  1.00  0.00
ATOM   1158  HN  LYS    71      10.816  -2.163  -5.131  1.00  0.00
ATOM   1159  CA  LYS    71       9.258  -0.761  -4.863  1.00  0.00
ATOM   1160  HA  LYS    71       8.988  -0.582  -3.832  1.00  0.00
ATOM   1161  CB  LYS    71      10.271   0.305  -5.297  1.00  0.00
ATOM   1162  HB1 LYS    71      11.076   0.332  -4.577  1.00  0.00
ATOM   1163  HB2 LYS    71      10.673   0.029  -6.261  1.00  0.00
ATOM   1164  CG  LYS    71       9.687   1.706  -5.409  1.00  0.00
ATOM   1165  HG1 LYS    71       9.956   2.267  -4.528  1.00  0.00
ATOM   1166  HG2 LYS    71       8.613   1.638  -5.482  1.00  0.00
ATOM   1167  CD  LYS    71      10.218   2.433  -6.634  1.00  0.00
ATOM   1168  HD1 LYS    71      11.033   1.863  -7.054  1.00  0.00
ATOM   1169  HD2 LYS    71       9.424   2.521  -7.360  1.00  0.00
ATOM   1170  CE  LYS    71      10.721   3.824  -6.282  1.00  0.00
ATOM   1171  HE1 LYS    71      11.466   3.737  -5.506  1.00  0.00
ATOM   1172  HE2 LYS    71       9.891   4.412  -5.919  1.00  0.00
ATOM   1173  NZ  LYS    71      11.323   4.511  -7.457  1.00  0.00
ATOM   1174  HZ1 LYS    71      10.580   4.970  -8.023  1.00  0.00
ATOM   1175  HZ2 LYS    71      11.823   3.823  -8.056  1.00  0.00
ATOM   1176  HZ3 LYS    71      12.000   5.234  -7.141  1.00  0.00
ATOM   1177  C   LYS    71       7.984  -0.678  -5.707  1.00  0.00
ATOM   1178  O   LYS    71       6.898  -1.000  -5.224  1.00  0.00
ATOM   1179  N   LYS    72       8.116  -0.244  -6.964  1.00  0.00
ATOM   1180  HN  LYS    72       9.002   0.015  -7.290  1.00  0.00
ATOM   1181  CA  LYS    72       6.963  -0.053  -7.846  1.00  0.00
ATOM   1182  HA  LYS    72       6.511   0.892  -7.580  1.00  0.00
ATOM   1183  CB  LYS    72       7.419   0.008  -9.305  1.00  0.00
ATOM   1184  HB1 LYS    72       8.261   0.680  -9.379  1.00  0.00
ATOM   1185  HB2 LYS    72       7.728  -0.979  -9.615  1.00  0.00
ATOM   1186  CG  LYS    72       6.339   0.491 -10.258  1.00  0.00
ATOM   1187  HG1 LYS    72       6.588   0.174 -11.260  1.00  0.00
ATOM   1188  HG2 LYS    72       5.394   0.057  -9.965  1.00  0.00
ATOM   1189  CD  LYS    72       6.214   2.005 -10.238  1.00  0.00
ATOM   1190  HD1 LYS    72       5.264   2.284 -10.669  1.00  0.00
ATOM   1191  HD2 LYS    72       6.261   2.347  -9.214  1.00  0.00
ATOM   1192  CE  LYS    72       7.329   2.466 -11.031  1.00  0.00
ATOM   1193  HE1 LYS    72       7.643   3.559 -10.908  1.00  0.00
ATOM   1194  HE2 LYS    72       8.160   1.981 -11.102  1.00  0.00
ATOM   1195  NZ  LYS    72       6.889   3.041 -12.403  1.00  0.00
ATOM   1196  HZ1 LYS    72       7.488   3.605 -12.775  1.00  0.00
ATOM   1197  HZ2 LYS    72       5.902   3.366 -12.386  1.00  0.00
ATOM   1198  HZ3 LYS    72       6.961   2.219 -13.027  1.00  0.00
ATOM   1199  C   LYS    72       5.915  -1.152  -7.680  1.00  0.00
ATOM   1200  O   LYS    72       4.723  -0.913  -7.869  1.00  0.00
ATOM   1201  N   LEU    73       6.357  -2.345  -7.305  1.00  0.00
ATOM   1202  HN  LEU    73       7.318  -2.480  -7.168  1.00  0.00
ATOM   1203  CA  LEU    73       5.446  -3.462  -7.101  1.00  0.00
ATOM   1204  HA  LEU    73       4.802  -3.527  -7.966  1.00  0.00
ATOM   1205  CB  LEU    73       6.231  -4.764  -6.964  1.00  0.00
ATOM   1206  HB1 LEU    73       6.470  -4.910  -5.922  1.00  0.00
ATOM   1207  HB2 LEU    73       7.162  -4.656  -7.512  1.00  0.00
ATOM   1208  CG  LEU    73       5.508  -6.014  -7.466  1.00  0.00
ATOM   1209  HG  LEU    73       4.553  -6.094  -6.966  1.00  0.00
ATOM   1210  CD1 LEU    73       6.315  -7.262  -7.145  1.00  0.00
ATOM   1211  HD11 LEU    73       6.321  -7.421  -6.076  1.00  0.00
ATOM   1212  HD12 LEU    73       7.328  -7.136  -7.496  1.00  0.00
ATOM   1213  HD13 LEU    73       5.868  -8.115  -7.631  1.00  0.00
ATOM   1214  CD2 LEU    73       5.247  -5.915  -8.961  1.00  0.00
ATOM   1215  HD21 LEU    73       4.982  -6.889  -9.345  1.00  0.00
ATOM   1216  HD22 LEU    73       6.138  -5.562  -9.459  1.00  0.00
ATOM   1217  HD23 LEU    73       4.437  -5.224  -9.140  1.00  0.00
ATOM   1218  C   LEU    73       4.587  -3.247  -5.861  1.00  0.00
ATOM   1219  O   LEU    73       3.375  -3.053  -5.958  1.00  0.00
ATOM   1220  N   PHE    74       5.218  -3.316  -4.693  1.00  0.00
ATOM   1221  HN  PHE    74       6.184  -3.474  -4.678  1.00  0.00
ATOM   1222  CA  PHE    74       4.513  -3.144  -3.434  1.00  0.00
ATOM   1223  HA  PHE    74       3.549  -3.622  -3.526  1.00  0.00
ATOM   1224  CB  PHE    74       5.290  -3.809  -2.305  1.00  0.00
ATOM   1225  HB1 PHE    74       6.174  -3.224  -2.095  1.00  0.00
ATOM   1226  HB2 PHE    74       5.587  -4.799  -2.614  1.00  0.00
ATOM   1227  CG  PHE    74       4.504  -3.929  -1.033  1.00  0.00
ATOM   1228  CD1 PHE    74       4.062  -5.163  -0.585  1.00  0.00
ATOM   1229  HD1 PHE    74       4.271  -6.043  -1.166  1.00  0.00
ATOM   1230  CD2 PHE    74       4.223  -2.807  -0.277  1.00  0.00
ATOM   1231  HD2 PHE    74       4.578  -1.842  -0.610  1.00  0.00
ATOM   1232  CE1 PHE    74       3.350  -5.272   0.593  1.00  0.00
ATOM   1233  HE1 PHE    74       3.006  -6.238   0.930  1.00  0.00
ATOM   1234  CE2 PHE    74       3.518  -2.911   0.903  1.00  0.00
ATOM   1235  HE2 PHE    74       3.316  -2.029   1.489  1.00  0.00
ATOM   1236  CZ  PHE    74       3.087  -4.144   1.342  1.00  0.00
ATOM   1237  HZ  PHE    74       2.524  -4.223   2.257  1.00  0.00
ATOM   1238  C   PHE    74       4.300  -1.670  -3.113  1.00  0.00
ATOM   1239  O   PHE    74       3.172  -1.236  -2.879  1.00  0.00
ATOM   1240  N   MET    75       5.392  -0.902  -3.095  1.00  0.00
ATOM   1241  HN  MET    75       6.262  -1.309  -3.281  1.00  0.00
ATOM   1242  CA  MET    75       5.324   0.529  -2.788  1.00  0.00
ATOM   1243  HA  MET    75       5.190   0.628  -1.721  1.00  0.00
ATOM   1244  CB  MET    75       6.617   1.240  -3.192  1.00  0.00
ATOM   1245  HB1 MET    75       6.403   2.289  -3.330  1.00  0.00
ATOM   1246  HB2 MET    75       6.964   0.834  -4.124  1.00  0.00
ATOM   1247  CG  MET    75       7.738   1.120  -2.171  1.00  0.00
ATOM   1248  HG1 MET    75       8.668   1.379  -2.652  1.00  0.00
ATOM   1249  HG2 MET    75       7.546   1.818  -1.373  1.00  0.00
ATOM   1250  SD  MET    75       7.907  -0.529  -1.461  1.00  0.00
ATOM   1251  CE  MET    75       7.869  -0.183   0.288  1.00  0.00
ATOM   1252  HE1 MET    75       8.136  -1.036   0.851  1.00  0.00
ATOM   1253  HE2 MET    75       6.875   0.161   0.564  1.00  0.00
ATOM   1254  HE3 MET    75       8.569   0.638   0.506  1.00  0.00
ATOM   1255  C   MET    75       4.136   1.176  -3.488  1.00  0.00
ATOM   1256  O   MET    75       3.495   2.073  -2.942  1.00  0.00
ATOM   1257  N   ALA    76       3.826   0.692  -4.687  1.00  0.00
ATOM   1258  HN  ALA    76       4.346  -0.055  -5.060  1.00  0.00
ATOM   1259  CA  ALA    76       2.659   1.177  -5.404  1.00  0.00
ATOM   1260  HA  ALA    76       2.666   2.259  -5.381  1.00  0.00
ATOM   1261  CB  ALA    76       2.669   0.723  -6.853  1.00  0.00
ATOM   1262  HB1 ALA    76       3.441   1.251  -7.393  1.00  0.00
ATOM   1263  HB2 ALA    76       1.706   0.935  -7.300  1.00  0.00
ATOM   1264  HB3 ALA    76       2.858  -0.338  -6.895  1.00  0.00
ATOM   1265  C   ALA    76       1.409   0.682  -4.714  1.00  0.00
ATOM   1266  O   ALA    76       0.613   1.472  -4.236  1.00  0.00
ATOM   1267  N   ASP    77       1.266  -0.640  -4.600  1.00  0.00
ATOM   1268  HN  ASP    77       1.977  -1.214  -4.989  1.00  0.00
ATOM   1269  CA  ASP    77       0.136  -1.260  -3.941  1.00  0.00
ATOM   1270  HA  ASP    77      -0.692  -1.239  -4.637  1.00  0.00
ATOM   1271  CB  ASP    77       0.454  -2.714  -3.586  1.00  0.00
ATOM   1272  HB1 ASP    77       1.280  -2.736  -2.891  1.00  0.00
ATOM   1273  HB2 ASP    77      -0.413  -3.164  -3.124  1.00  0.00
ATOM   1274  CG  ASP    77       0.831  -3.537  -4.802  1.00  0.00
ATOM   1275  OD1 ASP    77       0.295  -3.261  -5.896  1.00  0.00
ATOM   1276  OD2 ASP    77       1.666  -4.455  -4.661  1.00  0.00
ATOM   1277  C   ASP    77      -0.266  -0.491  -2.685  1.00  0.00
ATOM   1278  O   ASP    77      -1.436  -0.169  -2.498  1.00  0.00
ATOM   1279  N   LEU    78       0.718  -0.155  -1.857  1.00  0.00
ATOM   1280  HN  LEU    78       1.639  -0.417  -2.071  1.00  0.00
ATOM   1281  CA  LEU    78       0.466   0.617  -0.649  1.00  0.00
ATOM   1282  HA  LEU    78      -0.294   0.104  -0.077  1.00  0.00
ATOM   1283  CB  LEU    78       1.744   0.724   0.185  1.00  0.00
ATOM   1284  HB1 LEU    78       1.931   1.768   0.378  1.00  0.00
ATOM   1285  HB2 LEU    78       2.562   0.336  -0.402  1.00  0.00
ATOM   1286  CG  LEU    78       1.726  -0.016   1.529  1.00  0.00
ATOM   1287  HG  LEU    78       2.742  -0.221   1.827  1.00  0.00
ATOM   1288  CD1 LEU    78       0.998  -1.347   1.413  1.00  0.00
ATOM   1289  HD11 LEU    78      -0.066  -1.174   1.360  1.00  0.00
ATOM   1290  HD12 LEU    78       1.222  -1.955   2.277  1.00  0.00
ATOM   1291  HD13 LEU    78       1.327  -1.855   0.521  1.00  0.00
ATOM   1292  CD2 LEU    78       1.094   0.844  2.606  1.00  0.00
ATOM   1293  HD21 LEU    78       1.126   1.880  2.303  1.00  0.00
ATOM   1294  HD22 LEU    78       1.641   0.721  3.529  1.00  0.00
ATOM   1295  HD23 LEU    78       0.068   0.541  2.752  1.00  0.00
ATOM   1296  C   LEU    78      -0.045   2.009 -1.009  1.00  0.00
ATOM   1297  O   LEU    78      -1.164   2.385 -0.657  1.00  0.00
ATOM   1298  N   GLN    79       0.780   2.760 -1.731  1.00  0.00
ATOM   1299  HN  GLN    79       1.649   2.393 -1.995  1.00  0.00
ATOM   1300  CA  GLN    79       0.410   4.097 -2.184  1.00  0.00
ATOM   1301  HA  GLN    79       0.357   4.744 -1.321  1.00  0.00
ATOM   1302  CB  GLN    79       1.478   4.621 -3.154  1.00  0.00
ATOM   1303  HB1 GLN    79       1.727   3.833 -3.850  1.00  0.00
ATOM   1304  HB2 GLN    79       2.362   4.879 -2.591  1.00  0.00
ATOM   1305  CG  GLN    79       1.052   5.840 -3.958  1.00  0.00
ATOM   1306  HG1 GLN    79       0.674   5.507 -4.911  1.00  0.00
ATOM   1307  HG2 GLN    79       0.270   6.356 -3.421  1.00  0.00
ATOM   1308  CD  GLN    79       2.194   6.807 -4.202  1.00  0.00
ATOM   1309  OE1 GLN    79       2.996   7.551 -3.307  1.00  0.00
ATOM   1310  NE2 GLN    79       2.722   6.801 -5.420  1.00  0.00
ATOM   1311  HE21 GLN    79       3.463   7.416 -5.607  1.00  0.00
ATOM   1312  HE22 GLN    79       2.350   6.182 -6.083  1.00  0.00
ATOM   1313  C   GLN    79      -0.953   4.061 -2.870  1.00  0.00
ATOM   1314  O   GLN    79      -1.745   4.997 -2.768  1.00  0.00
ATOM   1315  N   ARG    80      -1.205   2.961 -3.563  1.00  0.00
ATOM   1316  HN  ARG    80      -0.522   2.263 -3.602  1.00  0.00
ATOM   1317  CA  ARG    80      -2.439   2.758 -4.287  1.00  0.00
ATOM   1318  HA  ARG    80      -2.705   3.686 -4.766  1.00  0.00
ATOM   1319  CB  ARG    80      -2.211   1.682 -5.361  1.00  0.00
ATOM   1320  HB1 ARG    80      -1.153   1.505 -5.449  1.00  0.00
ATOM   1321  HB2 ARG    80      -2.686   0.767 -5.059  1.00  0.00
ATOM   1322  CG  ARG    80      -2.725   2.063 -6.740  1.00  0.00
ATOM   1323  HG1 ARG    80      -2.057   2.795 -7.171  1.00  0.00
ATOM   1324  HG2 ARG    80      -2.742   1.180 -7.363  1.00  0.00
ATOM   1325  CD  ARG    80      -4.122   2.649 -6.682  1.00  0.00
ATOM   1326  HD1 ARG    80      -4.422   2.735 -5.653  1.00  0.00
ATOM   1327  HD2 ARG    80      -4.792   1.982 -7.193  1.00  0.00
ATOM   1328  NE  ARG    80      -4.186   3.966 -7.310  1.00  0.00
ATOM   1329  HE  ARG    80      -3.338   4.403 -7.534  1.00  0.00
ATOM   1330  CZ  ARG    80      -5.322   4.595 -7.594  1.00  0.00
ATOM   1331  NH1 ARG    80      -6.486   4.030 -7.305  1.00  0.00
ATOM   1332  HH11 ARG    80      -7.339   4.505 -7.519  1.00  0.00
ATOM   1333  HH12 ARG    80      -6.509   3.129 -6.872  1.00  0.00
ATOM   1334  NH2 ARG    80      -5.294   5.790 -8.168  1.00  0.00
ATOM   1335  HH21 ARG    80      -4.418   6.219 -8.386  1.00  0.00
ATOM   1336  HH22 ARG    80      -6.149   6.263 -8.380  1.00  0.00
ATOM   1337  C   ARG    80      -3.562   2.353 -3.329  1.00  0.00
ATOM   1338  O   ARG    80      -4.715   2.740 -3.513  1.00  0.00
ATOM   1339  N   VAL    81      -3.210   1.620 -2.273  1.00  0.00
ATOM   1340  HN  VAL    81      -2.271   1.367 -2.155  1.00  0.00
ATOM   1341  CA  VAL    81      -4.189   1.231 -1.261  1.00  0.00
ATOM   1342  HA  VAL    81      -4.947   0.630 -1.742  1.00  0.00
ATOM   1343  CB  VAL    81      -3.543   0.387 -0.129  1.00  0.00
ATOM   1344  HB  VAL    81      -2.648   0.893   0.201  1.00  0.00
ATOM   1345  CG1 VAL    81      -3.147  -0.988 -0.645  1.00  0.00
ATOM   1346  HG11 VAL    81      -2.073  -1.089 -0.614  1.00  0.00
ATOM   1347  HG12 VAL    81      -3.491  -1.105 -1.661  1.00  0.00
ATOM   1348  HG13 VAL    81      -3.597  -1.750 -0.023  1.00  0.00
ATOM   1349  CG2 VAL    81      -4.476   0.247  1.070  1.00  0.00
ATOM   1350  HG21 VAL    81      -5.364  -0.291   0.774  1.00  0.00
ATOM   1351  HG22 VAL    81      -4.752   1.228  1.429  1.00  0.00
ATOM   1352  HG23 VAL    81      -3.972  -0.295   1.857  1.00  0.00
ATOM   1353  C   VAL    81      -4.844   2.481 -0.674  1.00  0.00
ATOM   1354  O   VAL    81      -6.050   2.507 -0.427  1.00  0.00
ATOM   1355  N   PHE    82      -4.037   3.515 -0.459  1.00  0.00
ATOM   1356  HN  PHE    82      -3.086   3.434 -0.684  1.00  0.00
ATOM   1357  CA  PHE    82      -4.533   4.774  0.080  1.00  0.00
ATOM   1358  HA  PHE    82      -5.269   4.545  0.837  1.00  0.00
ATOM   1359  CB  PHE    82      -3.390   5.572  0.717  1.00  0.00
ATOM   1360  HB1 PHE    82      -2.807   6.034 -0.065  1.00  0.00
ATOM   1361  HB2 PHE    82      -3.810   6.342  1.348  1.00  0.00
ATOM   1362  CG  PHE    82      -2.455   4.746  1.561  1.00  0.00
ATOM   1363  CD1 PHE    82      -2.850   3.520  2.077  1.00  0.00
ATOM   1364  HD1 PHE    82      -3.841   3.149  1.861  1.00  0.00
ATOM   1365  CD2 PHE    82      -1.180   5.209  1.850  1.00  0.00
ATOM   1366  HD2 PHE    82      -0.862   6.163  1.457  1.00  0.00
ATOM   1367  CE1 PHE    82      -1.988   2.768  2.853  1.00  0.00
ATOM   1368  HE1 PHE    82      -2.307   1.815  3.248  1.00  0.00
ATOM   1369  CE2 PHE    82      -0.316   4.462  2.627  1.00  0.00
ATOM   1370  HE2 PHE    82       0.675   4.834  2.862  1.00  0.00
ATOM   1371  CZ  PHE    82      -0.721   3.242  3.131  1.00  0.00
ATOM   1372  HZ  PHE    82      -0.047   2.659  3.741  1.00  0.00
ATOM   1373  C   PHE    82      -5.194   5.601 -1.016  1.00  0.00
ATOM   1374  O   PHE    82      -6.353   5.997 -0.895  1.00  0.00
ATOM   1375  N   THR    83      -4.450   5.849 -2.089  1.00  0.00
ATOM   1376  HN  THR    83      -3.536   5.499 -2.129  1.00  0.00
ATOM   1377  CA  THR    83      -4.968   6.616 -3.215  1.00  0.00
ATOM   1378  HA  THR    83      -5.151   7.624 -2.875  1.00  0.00
ATOM   1379  CB  THR    83      -3.941   6.649 -4.350  1.00  0.00
ATOM   1380  HB  THR    83      -3.649   5.637 -4.588  1.00  0.00
ATOM   1381  OG1 THR    83      -2.784   7.365 -3.958  1.00  0.00
ATOM   1382  HG1 THR    83      -2.246   6.813 -3.382  1.00  0.00
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ATOM   1383  CG2 THR  83      -4.464   7.286  -5.619  1.00  0.00
ATOM   1384 HG21 THR  83      -3.654   7.404  -6.323  1.00  0.00
ATOM   1385 HG22 THR  83      -4.884   8.255  -5.389  1.00  0.00
ATOM   1386 HG23 THR  83      -5.228   6.656  -6.049  1.00  0.00
ATOM   1387  C   THR  83      -6.278   6.017  -3.711  1.00  0.00
ATOM   1388  O   THR  83      -7.221   6.740  -4.033  1.00  0.00
ATOM   1389  N   ASN  84      -6.333   4.690  -3.756  1.00  0.00
ATOM   1390  HN  ASN  84      -5.550   4.170  -3.476  1.00  0.00
ATOM   1391  CA  ASN  84      -7.533   3.987  -4.190  1.00  0.00
ATOM   1392  HA  ASN  84      -7.822   4.381  -5.153  1.00  0.00
ATOM   1393  CB  ASN  84      -7.250   2.491  -4.321  1.00  0.00
ATOM   1394  HB1 ASN  84      -6.457   2.342  -5.039  1.00  0.00
ATOM   1395  HB2 ASN  84      -6.939   2.107  -3.362  1.00  0.00
ATOM   1396  CG  ASN  84      -8.464   1.707  -4.778  1.00  0.00
ATOM   1397  OD1 ASN  84      -9.459   2.282  -5.218  1.00  0.00
ATOM   1398  ND2 ASN  84      -8.388   0.385  -4.672  1.00  0.00
ATOM   1399 HD21 ASN  84      -7.564  -0.004  -4.312  1.00  0.00
ATOM   1400 HD22 ASN  84      -9.158  -0.147  -4.960  1.00  0.00
ATOM   1401  C   ASN  84      -8.670   4.212  -3.201  1.00  0.00
ATOM   1402  O   ASN  84      -9.656   4.879  -3.514  1.00  0.00
ATOM   1403  N   CYS  85      -8.520   3.657  -2.003  1.00  0.00
ATOM   1404  HN  CYS  85      -7.708   3.142  -1.812  1.00  0.00
ATOM   1405  CA  CYS  85      -9.526   3.808  -0.961  1.00  0.00
ATOM   1406  HA  CYS  85     -10.414   3.280  -1.276  1.00  0.00
ATOM   1407  CB  CYS  85      -9.028   3.205   0.354  1.00  0.00
ATOM   1408  HB1 CYS  85      -9.769   3.329   1.109  1.00  0.00
ATOM   1409  HB2 CYS  85      -8.132   3.724   0.665  1.00  0.00
ATOM   1410  SG  CYS  85      -8.635   1.443   0.257  1.00  0.00
ATOM   1411  HG  CYS  85      -9.362   0.955   0.652  1.00  0.00
ATOM   1412  C   CYS  85      -9.873   5.278  -0.759  1.00  0.00
ATOM   1413  O   CYS  85     -10.996   5.613  -0.398  1.00  0.00
ATOM   1414  N   LYS  86      -8.898   6.150  -0.993  1.00  0.00
ATOM   1415  HN  LYS  86      -8.021   5.820  -1.281  1.00  0.00
ATOM   1416  CA  LYS  86      -9.102   7.586  -0.840  1.00  0.00
ATOM   1417  HA  LYS  86      -9.725   7.741   0.029  1.00  0.00
ATOM   1418  CB  LYS  86      -7.758   8.290  -0.623  1.00  0.00
ATOM   1419  HB1 LYS  86      -7.355   7.984   0.330  1.00  0.00
ATOM   1420  HB2 LYS  86      -7.078   7.990  -1.405  1.00  0.00
ATOM   1421  CG  LYS  86      -7.853   9.807  -0.632  1.00  0.00
ATOM   1422  HG1 LYS  86      -8.858  10.091  -0.901  1.00  0.00
ATOM   1423  HG2 LYS  86      -7.625  10.178   0.356  1.00  0.00
ATOM   1424  CD  LYS  86      -6.882  10.424  -1.626  1.00  0.00
ATOM   1425  HD1 LYS  86      -7.437  11.020  -2.334  1.00  0.00
ATOM   1426  HD2 LYS  86      -6.363   9.633  -2.147  1.00  0.00
ATOM   1427  CE  LYS  86      -5.860  11.308  -0.930  1.00  0.00
ATOM   1428  HE1 LYS  86      -5.744  10.970   0.090  1.00  0.00
ATOM   1429  HE2 LYS  86      -4.916  11.221  -1.447  1.00  0.00
ATOM   1430  NZ  LYS  86      -6.276  12.738  -0.922  1.00  0.00
ATOM   1431  HZ1 LYS  86      -6.207  13.125   0.041  1.00  0.00
ATOM   1432  HZ2 LYS  86      -7.260  12.825  -1.249  1.00  0.00
ATOM   1433  HZ3 LYS  86      -5.663  13.292  -1.552  1.00  0.00
ATOM   1434  C   LYS  86      -9.805   8.175  -2.060  1.00  0.00
ATOM   1435  O   LYS  86     -10.579   9.126  -1.943  1.00  0.00
ATOM   1436  N   GLU  87      -9.518   7.615  -3.230  1.00  0.00
ATOM   1437  HN  GLU  87      -8.883   6.869  -3.259  1.00  0.00
ATOM   1438  CA  GLU  87     -10.101   8.103  -4.474  1.00  0.00
ATOM   1439  HA  GLU  87     -10.101   9.183  -4.435  1.00  0.00
ATOM   1440  CB  GLU  87      -9.256   7.649  -5.665  1.00  0.00
ATOM   1441  HB1 GLU  87      -9.884   7.607  -6.542  1.00  0.00
ATOM   1442  HB2 GLU  87      -8.869   6.662  -5.462  1.00  0.00
ATOM   1443  CG  GLU  87      -8.084   8.570  -5.963  1.00  0.00
ATOM   1444  HG1 GLU  87      -7.726   8.989  -6.033  1.00  0.00
ATOM   1445  HG2 GLU  87      -7.296   7.993  -6.424  1.00  0.00
ATOM   1446  CD  GLU  87      -8.460   9.707  -6.893  1.00  0.00
ATOM   1447  OE1 GLU  87      -9.484   9.583  -7.597  1.00  0.00
ATOM   1448  OE2 GLU  87      -7.732  10.721  -6.916  1.00  0.00
ATOM   1449  C   GLU  87     -11.539   7.621  -4.645  1.00  0.00
ATOM   1450  O   GLU  87     -12.422   8.397  -5.010  1.00  0.00
ATOM   1451  N   TYR  88     -11.769   6.338  -4.367  1.00  0.00
ATOM   1452  HN  TYR  88     -11.023   5.763  -4.109  1.00  0.00
ATOM   1453  CA  TYR  88     -13.100   5.757  -4.536  1.00  0.00
ATOM   1454  HA  TYR  88     -13.528   6.144  -5.449  1.00  0.00
ATOM   1455  CB  TYR  88     -13.000   4.234  -4.639  1.00  0.00
ATOM   1456  HB1 TYR  88     -12.032   3.971  -5.040  1.00  0.00
ATOM   1457  HB2 TYR  88     -13.104   3.806  -3.653  1.00  0.00
ATOM   1458  CG  TYR  88     -14.054   3.612  -5.527  1.00  0.00
ATOM   1459  CD1 TYR  88     -15.165   2.982  -4.982  1.00  0.00
ATOM   1460  HD1 TYR  88     -15.273   2.942  -3.908  1.00  0.00
ATOM   1461  CD2 TYR  88     -13.935   3.651  -6.911  1.00  0.00
ATOM   1462  HD2 TYR  88     -13.076   4.136  -7.350  1.00  0.00
ATOM   1463  CE1 TYR  88     -16.130   2.410  -5.790  1.00  0.00
ATOM   1464  HE1 TYR  88     -16.987   1.925  -5.347  1.00  0.00
ATOM   1465  CE2 TYR  88     -14.894   3.081  -7.726  1.00  0.00
ATOM   1466  HE2 TYR  88     -14.785   3.122  -8.800  1.00  0.00
ATOM   1467  CZ  TYR  88     -15.990   2.463  -7.161  1.00  0.00
ATOM   1468  OH  TYR  88     -16.947   1.893  -7.969  1.00  0.00
ATOM   1469  HH  TYR  88     -17.473   2.584  -8.178  1.00  0.00
ATOM   1470  C   TYR  88     -14.010   6.137  -3.368  1.00  0.00
ATOM   1471  O   TYR  88     -14.555   5.265  -2.691  1.00  0.00
ATOM   1472  N   ASN  89     -14.187   7.439  -3.150  1.00  0.00
ATOM   1473  HN  ASN  89     -13.727   8.087  -3.727  1.00  0.00
ATOM   1474  CA  ASN  89     -15.038   7.925  -2.070  1.00  0.00
ATOM   1475  HA  ASN  89     -15.682   7.102  -1.736  1.00  0.00
ATOM   1476  CB  ASN  89     -14.185   8.416  -0.899  1.00  0.00
ATOM   1477  HB1 ASN  89     -14.820   8.581  -0.042  1.00  0.00
ATOM   1478  HB2 ASN  89     -13.706   9.344  -1.173  1.00  0.00
ATOM   1479  CG  ASN  89     -13.111   7.419  -0.617  1.00  0.00
ATOM   1480  OD1 ASN  89     -12.001   7.796  -0.149  1.00  0.00
ATOM   1481  ND2 ASN  89     -13.444   6.136  -0.609  1.00  0.00
ATOM   1482 HD21 ASN  89     -12.769   5.467  -0.377  1.00  0.00
ATOM   1483 HD22 ASN  89     -14.348   5.910  -0.912  1.00  0.00
ATOM   1484  C   ASN  89     -15.944   9.048  -2.552  1.00  0.00
ATOM   1485  O   ASN  89     -15.701  10.222  -2.272  1.00  0.00
ATOM   1486  N   ALA  90     -16.997   8.680  -3.272  1.00  0.00
ATOM   1487  HN  ALA  90     -17.141   7.728  -3.456  1.00  0.00
ATOM   1488  CA  ALA  90     -17.954   9.655  -3.783  1.00  0.00
ATOM   1489  HA  ALA  90     -17.486  10.184  -4.599  1.00  0.00
ATOM   1490  CB  ALA  90     -19.185   8.946  -4.326  1.00  0.00
ATOM   1491  HB1 ALA  90     -19.210   7.944  -3.926  1.00  0.00
ATOM   1492  HB2 ALA  90     -19.128   8.901  -5.404  1.00  0.00
ATOM   1493  HB3 ALA  90     -20.072   9.490  -4.035  1.00  0.00
ATOM   1494  C   ALA  90     -18.356  10.662  -2.705  1.00  0.00
ATOM   1495  O   ALA  90     -18.383  11.868  -2.952  1.00  0.00
ATOM   1496  N   PRO  91     -18.657  10.179  -1.487  1.00  0.00
ATOM   1497  CA  PRO  91     -19.087  11.013  -0.381  1.00  0.00
ATOM   1498  HA  PRO  91     -19.505  11.951  -0.717  1.00  0.00
ATOM   1499  CB  PRO  91     -20.176  10.140   0.237  1.00  0.00
ATOM   1500  HB1 PRO  91     -20.271  10.369   1.289  1.00  0.00
ATOM   1501  HB2 PRO  91     -21.115  10.323  -0.263  1.00  0.00
ATOM   1502  CG  PRO  91     -19.704   8.730   0.022  1.00  0.00
ATOM   1503  HG1 PRO  91     -20.537   8.104  -0.258  1.00  0.00
ATOM   1504  HG2 PRO  91     -19.249   8.358   0.929  1.00  0.00
ATOM   1505  CD  PRO  91     -18.679   9.764  -1.094  1.00  0.00
ATOM   1506  HD1 PRO  91     -17.713   9.452  -0.724  1.00  0.00
ATOM   1507  HD2 PRO  91     -18.988   9.139  -1.919  1.00  0.00
ATOM   1508  C   PRO  91     -17.976  11.268   0.633  1.00  0.00
ATOM   1509  O   PRO  91     -18.242  11.671   1.766  1.00  0.00
ATOM   1510  N   GLU  92     -16.734  11.007   0.234  1.00  0.00
ATOM   1511  HN  GLU  92     -16.582  10.671  -0.674  1.00  0.00
ATOM   1512  CA  GLU  92     -15.596  11.174   1.132  1.00  0.00
ATOM   1513  HA  GLU  92     -14.728  10.745   0.654  1.00  0.00
ATOM   1514  CB  GLU  92     -15.340  12.658   1.408  1.00  0.00
ATOM   1515  HB1 GLU  92     -14.454  12.750   2.020  1.00  0.00
ATOM   1516  HB2 GLU  92     -16.183  13.062   1.949  1.00  0.00
ATOM   1517  CG  GLU  92     -15.139  13.487   0.150  1.00  0.00
ATOM   1518  HG1 GLU  92     -15.062  12.821  -0.696  1.00  0.00
ATOM   1519  HG2 GLU  92     -15.993  14.135   0.021  1.00  0.00
ATOM   1520  CD  GLU  92     -13.888  14.343   0.208  1.00  0.00
ATOM   1521  OE1 GLU  92     -13.118  14.335  -0.775  1.00  0.00
ATOM   1522  OE2 GLU  92     -13.679  15.021   1.236  1.00  0.00
ATOM   1523  C   GLU  92     -15.843  10.432   2.436  1.00  0.00
ATOM   1524  O   GLU  92     -15.529  10.925   3.519  1.00  0.00
ATOM   1525  N   SER  93     -16.427   9.248   2.313  1.00  0.00
ATOM   1526  HN  SER  93     -16.648   8.819   1.417  1.00  0.00
ATOM   1527  CA  SER  93     -16.725   8.412   3.463  1.00  0.00
ATOM   1528  HA  SER  93     -17.495   8.899   4.042  1.00  0.00
ATOM   1529  CB  SER  93     -17.234   7.048   2.986  1.00  0.00
ATOM   1530  HB1 SER  93     -17.222   6.350   3.809  1.00  0.00
ATOM   1531  HB2 SER  93     -18.243   7.152   2.615  1.00  0.00
ATOM   1532  OG  SER  93     -16.418   6.536   1.947  1.00  0.00
ATOM   1533  HG  SER  93     -16.849   6.678   1.101  1.00  0.00
ATOM   1534  C   SER  93     -15.490   8.232   4.335  1.00  0.00
ATOM   1535  O   SER  93     -14.447   8.833   4.082  1.00  0.00
ATOM   1536  N   GLU  94     -15.601   7.370   5.338  1.00  0.00
ATOM   1537  HN  GLU  94     -16.455   6.913   5.685  1.00  0.00
ATOM   1538  CA  GLU  94     -14.485   7.092   6.230  1.00  0.00
ATOM   1539  HA  GLU  94     -14.213   8.017   6.717  1.00  0.00
ATOM   1540  CB  GLU  94     -14.901   6.073   7.292  1.00  0.00
ATOM   1541  HB1 GLU  94     -14.489   5.109   7.031  1.00  0.00
ATOM   1542  HB2 GLU  94     -15.979   6.003   7.305  1.00  0.00
ATOM   1543  CG  GLU  94     -14.430   6.427   8.693  1.00  0.00
ATOM   1544  HG1 GLU  94     -13.574   7.082   8.616  1.00  0.00
ATOM   1545  HG2 GLU  94     -15.229   6.939   9.209  1.00  0.00
ATOM   1546  CD  GLU  94     -14.035   5.207   9.502  1.00  0.00
ATOM   1547  OE1 GLU  94     -13.155   5.336  10.379  1.00  0.00
ATOM   1548  OE2 GLU  94     -14.604   4.123   9.257  1.00  0.00
ATOM   1549  C   GLU  94     -13.274   6.569   5.457  1.00  0.00
ATOM   1550  O   GLU  94     -12.160   6.551   5.979  1.00  0.00
ATOM   1551  N   TYR  95     -13.493   6.137   4.214  1.00  0.00
ATOM   1552  HN  TYR  95     -14.397   6.168   3.841  1.00  0.00
ATOM   1553  CA  TYR  95     -12.412   5.611   3.393  1.00  0.00
ATOM   1554  HA  TYR  95     -11.977   4.775   3.916  1.00  0.00
ATOM   1555  CB  TYR  95     -12.947   5.121   2.045  1.00  0.00
ATOM   1556  HB1 TYR  95     -13.630   5.870   1.651  1.00  0.00
ATOM   1557  HB2 TYR  95     -12.119   5.016   1.365  1.00  0.00
ATOM   1558  CG  TYR  95     -13.678   3.807   2.104  1.00  0.00
ATOM   1559  CD1 TYR  95     -13.724   2.972   0.996  1.00  0.00
ATOM   1560  HD1 TYR  95     -13.227   3.279   0.087  1.00  0.00
ATOM   1561  CD2 TYR  95     -14.325   3.394   3.263  1.00  0.00
ATOM   1562  HD2 TYR  95     -14.303   4.030   4.132  1.00  0.00
ATOM   1563  CE1 TYR  95     -14.390   1.762   1.040  1.00  0.00
ATOM   1564  HE1 TYR  95     -14.413   1.126   0.167  1.00  0.00
ATOM   1565  CE2 TYR  95     -14.994   2.187   3.314  1.00  0.00
ATOM   1566  HE2 TYR  95     -15.487   1.884   4.227  1.00  0.00
ATOM   1567  CZ  TYR  95     -15.023   1.374   2.202  1.00  0.00
ATOM   1568  OH  TYR  95     -15.687   0.170   2.250  1.00  0.00
ATOM   1569  HH  TYR  95     -15.095  -0.634   1.974  1.00  0.00
ATOM   1570  C   TYR  95     -11.338   6.671   3.177  1.00  0.00
ATOM   1571  O   TYR  95     -10.170   6.352   2.951  1.00  0.00
ATOM   1572  N   TYR  96     -11.743   7.934   3.243  1.00  0.00
ATOM   1573  HN  TYR  96     -12.686   8.125   3.432  1.00  0.00
ATOM   1574  CA  TYR  96     -10.816   9.045   3.073  1.00  0.00
ATOM   1575  HA  TYR  96     -10.140   8.795   2.268  1.00  0.00
ATOM   1576  CB  TYR  96     -11.579  10.321   2.712  1.00  0.00
ATOM   1577  HB1 TYR  96     -12.376  10.073   2.027  1.00  0.00
ATOM   1578  HB2 TYR  96     -12.001  10.745   3.611  1.00  0.00
ATOM   1579  CG  TYR  96     -10.717  11.378   2.060  1.00  0.00
ATOM   1580  CD1 TYR  96     -10.257  11.219   0.759  1.00  0.00
ATOM   1581  HD1 TYR  96     -10.524  10.326   0.213  1.00  0.00
ATOM   1582  CD2 TYR  96     -10.364  12.533   2.745  1.00  0.00
ATOM   1583  HD2 TYR  96     -10.714  12.672   3.758  1.00  0.00
ATOM   1584  CE1 TYR  96      -9.471  12.183   0.159  1.00  0.00
ATOM   1585  HE1 TYR  96      -9.120  12.039  -0.852  1.00  0.00
ATOM   1586  CE2 TYR  96      -9.576  13.501   2.152  1.00  0.00
ATOM   1587  HE2 TYR  96      -9.312  14.393   2.701  1.00  0.00
ATOM   1588  CZ  TYR  96      -9.131  13.320   0.859  1.00  0.00
ATOM   1589  OH  TYR  96      -8.347  14.282   0.265  1.00  0.00
ATOM   1590  HH  TYR  96      -8.832  14.690  -0.456  1.00  0.00
ATOM   1591  C   TYR  96     -10.009   9.267   4.346  1.00  0.00
ATOM   1592  O   TYR  96      -8.884   9.764   4.303  1.00  0.00
ATOM   1593  N   LYS  97     -10.593   8.888   5.478  1.00  0.00
ATOM   1594  HN  LYS  97     -11.496   8.503   5.445  1.00  0.00
ATOM   1595  CA  LYS  97      -9.917   9.050   6.771  1.00  0.00
ATOM   1596  HA  LYS  97      -9.515  10.043   6.806  1.00  0.00
ATOM   1597  CB  LYS  97     -10.960   8.901   7.898  1.00  0.00
ATOM   1598  HB1 LYS  97     -11.380   7.906   7.859  1.00  0.00
ATOM   1599  HB2 LYS  97     -10.457   9.033   8.845  1.00  0.00
ATOM   1600  CG  LYS  97     -12.100   9.903   7.820  1.00  0.00
ATOM   1601  HG1 LYS  97     -12.840   9.537   7.124  1.00  0.00
ATOM   1602  HG2 LYS  97     -11.711  10.849   7.473  1.00  0.00
ATOM   1603  CD  LYS  97     -12.756  10.107   9.176  1.00  0.00
ATOM   1604  HD1 LYS  97     -13.665  10.674   9.042  1.00  0.00
ATOM   1605  HD2 LYS  97     -12.990   9.142   9.601  1.00  0.00
ATOM   1606  CE  LYS  97     -11.842  10.857  10.131  1.00  0.00
ATOM   1607  HE1 LYS  97     -10.927  11.105   9.614  1.00  0.00
ATOM   1608  HE2 LYS  97     -11.618  10.218  10.972  1.00  0.00
ATOM   1609  NZ  LYS  97     -12.471  12.211  10.629  1.00  0.00
ATOM   1610  HZ1 LYS  97     -11.831  12.917  10.476  1.00  0.00
ATOM   1611  HZ2 LYS  97     -12.672  12.031  11.646  1.00  0.00
ATOM   1612  HZ3 LYS  97     -13.362  12.289  10.123  1.00  0.00
ATOM   1613  C   LYS  97      -8.816   8.031   6.955  1.00  0.00
ATOM   1614  O   LYS  97      -7.664   8.395   7.189  1.00  0.00
ATOM   1615  N   CYS  98      -9.167   6.753   6.861  1.00  0.00
ATOM   1616  HN  CYS  98     -10.105   6.529   6.684  1.00  0.00
ATOM   1617  CA  CYS  98      -8.203   5.671   7.039  1.00  0.00
ATOM   1618  HA  CYS  98      -7.970   5.609   8.092  1.00  0.00
ATOM   1619  CB  CYS  98      -8.816   4.348   6.588  1.00  0.00
ATOM   1620  HB1 CYS  98      -8.039   3.600   6.531  1.00  0.00
ATOM   1621  HB2 CYS  98      -9.554   4.040   7.311  1.00  0.00
ATOM   1622  SG  CYS  98      -9.627   4.426   4.976  1.00  0.00
ATOM   1623  HG  CYS  98     -10.366   5.034   5.045  1.00  0.00
ATOM   1624  C   CYS  98      -6.914   5.931   6.268  1.00  0.00
ATOM   1625  O   CYS  98      -5.817   5.796   6.814  1.00  0.00
ATOM   1626  N   ALA  99      -7.045   6.278   4.991  1.00  0.00
ATOM   1627  HN  ALA  99      -7.933   6.375   4.607  1.00  0.00
ATOM   1628  CA  ALA  99      -5.885   6.551   4.158  1.00  0.00
ATOM   1629  HA  ALA  99      -5.339   5.629   4.029  1.00  0.00
ATOM   1630  CB  ALA  99      -6.319   7.042   2.785  1.00  0.00
ATOM   1631  HB1 ALA  99      -6.855   6.355   2.275  1.00  0.00
ATOM   1632  HB2 ALA  99      -5.448   7.317   2.209  1.00  0.00
ATOM   1633  HB3 ALA  99      -6.963   7.902   2.897  1.00  0.00
ATOM   1634  C   ALA  99      -4.977   7.570   4.828  1.00  0.00
ATOM   1635  O   ALA  99      -3.764   7.398   4.871  1.00  0.00
ATOM   1636  N   ASN 100      -5.581   8.613   5.379  1.00  0.00
ATOM   1637  HN  ASN 100      -6.555   8.685   5.321  1.00  0.00
ATOM   1638  CA  ASN 100      -4.826   9.660   6.084  1.00  0.00
ATOM   1639  HA  ASN 100      -4.202  10.142   5.316  1.00  0.00
ATOM   1640  CB  ASN 100      -5.778  10.695   6.658  1.00  0.00
ATOM   1641  HB1 ASN 100      -6.720  10.660   6.130  1.00  0.00
ATOM   1642  HB2 ASN 100      -5.943  10.459   7.699  1.00  0.00
ATOM   1643  CG  ASN 100      -5.230  12.106   6.568  1.00  0.00
ATOM   1644  OD1 ASN 100      -5.097  12.798   7.577  1.00  0.00
ATOM   1645  ND2 ASN 100      -4.910  12.541   5.354  1.00  0.00
ATOM   1646 HD21 ASN 100      -4.553  13.449   5.267  1.00  0.00
ATOM   1647 HD22 ASN 100      -5.042  11.934   4.595  1.00  0.00
ATOM   1648  C   ASN 100      -3.935   9.073   7.144  1.00  0.00
ATOM   1649  O   ASN 100      -2.862   9.602   7.434  1.00  0.00
ATOM   1650  N   ILE 101      -4.386   7.975   7.743  1.00  0.00
ATOM   1651  HN  ILE 101      -5.248   7.599   7.467  1.00  0.00
ATOM   1652  CA  ILE 101      -3.630   7.318   8.803  1.00  0.00
ATOM   1653  HA  ILE 101      -3.193   8.088   9.422  1.00  0.00
ATOM   1654  CB  ILE 101      -4.541   6.453   9.691  1.00  0.00
ATOM   1655  HB  ILE 101      -4.890   5.616   9.105  1.00  0.00
ATOM   1656 CG1  ILE 101      -5.743   7.274  10.166  1.00  0.00
ATOM   1657 HG11 ILE 101      -6.325   7.575   9.308  1.00  0.00
ATOM   1658 HG12 ILE 101      -5.387   8.153  10.682  1.00  0.00
ATOM   1659 CG2  ILE 101      -3.761   5.909  10.879  1.00  0.00
ATOM   1660 HG21 ILE 101      -4.431   5.373  11.534  1.00  0.00
ATOM   1661 HG22 ILE 101      -3.308   6.727  11.418  1.00  0.00
ATOM   1662 HG23 ILE 101      -2.990   9.240  10.926  1.00  0.00
ATOM   1663  CD1  ILE 101      -6.688   6.823  11.107  1.00  0.00
ATOM   1664 HD11 ILE 101      -7.168   7.226  11.749  1.00  0.00
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ATOM   1665 HD12 ILE   101      -6.075   5.862  11.709  1.00  0.00
ATOM   1666 HD13 ILE   101      -7.384   5.966  10.534  1.00  0.00
ATOM   1667  C   ILE   101      -2.511   6.457   8.226  1.00  0.00
ATOM   1668  O   ILE   101      -1.335   6.807   8.332  1.00  0.00
ATOM   1669  N   LEU   102      -2.876   5.343   7.590  1.00  0.00
ATOM   1670  HN  LEU   102      -3.829   5.117   7.527  1.00  0.00
ATOM   1671  CA  LEU   102      -1.886   4.457   6.972  1.00  0.00
ATOM   1672  HA  LEU   102      -1.350   3.953   7.761  1.00  0.00
ATOM   1673  CB  LEU   102      -2.569   3.416   6.082  1.00  0.00
ATOM   1674  HB1 LEU   102      -3.620   3.443   6.283  1.00  0.00
ATOM   1675  HB2 LEU   102      -2.408   3.700   5.053  1.00  0.00
ATOM   1676  CG  LEU   102      -2.083   1.971   6.260  1.00  0.00
ATOM   1677  HG  LEU   102      -2.423   1.382   5.420  1.00  0.00
ATOM   1678  CD1 LEU   102      -2.676   1.364   7.523  1.00  0.00
ATOM   1679 HD11 LEU   102      -1.943   1.395   8.316  1.00  0.00
ATOM   1680 HD12 LEU   102      -2.958   0.338   7.332  1.00  0.00
ATOM   1681 HD13 LEU   102      -3.549   1.928   7.618  1.00  0.00
ATOM   1682  CD2 LEU   102      -0.559   1.903   6.290  1.00  0.00
ATOM   1683 HD21 LEU   102      -0.147   2.788   5.827  1.00  0.00
ATOM   1684 HD22 LEU   102      -0.224   1.027   5.749  1.00  0.00
ATOM   1685 HD23 LEU   102      -0.220   1.841   7.313  1.00  0.00
ATOM   1686  C   LEU   102      -0.897   5.265   6.139  1.00  0.00
ATOM   1687  O   LEU   102       0.301   4.991   6.137  1.00  0.00
ATOM   1688  N   GLU   103      -1.414   6.266   5.433  1.00  0.00
ATOM   1689  HN  GLU   103      -2.377   6.439   5.484  1.00  0.00
ATOM   1690  CA  GLU   103      -0.581   7.132   4.613  1.00  0.00
ATOM   1691  HA  GLU   103      -0.056   6.514   3.900  1.00  0.00
ATOM   1692  CB  GLU   103      -1.446   8.165   3.857  1.00  0.00
ATOM   1693  HB1 GLU   103      -1.912   8.808   4.572  1.00  0.00
ATOM   1694  HB2 GLU   103      -2.220   7.612   3.320  1.00  0.00
ATOM   1695  CG  GLU   103      -0.670   8.991   2.860  1.00  0.00
ATOM   1696  HG1 GLU   103      -1.083   8.832   1.874  1.00  0.00
ATOM   1697  HG2 GLU   103       0.364   8.680   2.871  1.00  0.00
ATOM   1698  CD  GLU   103      -0.734  10.472   3.178  1.00  0.00
ATOM   1699  OE1 GLU   103      -1.856  10.996   3.342  1.00  0.00
ATOM   1700  OE2 GLU   103       0.337  11.108   3.264  1.00  0.00
ATOM   1701  C   GLU   103       0.439   7.858   5.478  1.00  0.00
ATOM   1702  O   GLU   103       1.644   7.658   5.334  1.00  0.00
ATOM   1703  N   LYS   104      -0.052   8.675   6.405  1.00  0.00
ATOM   1704  HN  LYS   104      -1.024   8.786   6.480  1.00  0.00
ATOM   1705  CA  LYS   104       0.821   9.417   7.306  1.00  0.00
ATOM   1706  HA  LYS   104       1.329  10.172   6.725  1.00  0.00
ATOM   1707  CB  LYS   104      -0.003  10.100   8.399  1.00  0.00
ATOM   1708  HB1 LYS   104      -0.949   9.589   8.492  1.00  0.00
ATOM   1709  HB2 LYS   104       0.530  10.024   9.335  1.00  0.00
ATOM   1710  CG  LYS   104      -0.278  11.569   8.125  1.00  0.00
ATOM   1711  HG1 LYS   104       0.635  12.128   8.261  1.00  0.00
ATOM   1712  HG2 LYS   104      -1.026  11.920   8.820  1.00  0.00
ATOM   1713  CD  LYS   104      -0.762  11.786   6.708  1.00  0.00
ATOM   1714  HD1 LYS   104      -0.960  10.824   6.248  1.00  0.00
ATOM   1715  HD2 LYS   104      -0.031  12.322   6.147  1.00  0.00
ATOM   1716  CE  LYS   104      -2.073  12.589   6.695  1.00  0.00
ATOM   1717  HE1 LYS   104      -2.601  12.384   5.775  1.00  0.00
ATOM   1718  HE2 LYS   104      -2.680  12.283   7.534  1.00  0.00
ATOM   1719  NZ  LYS   104      -1.817  14.053   6.791  1.00  0.00
ATOM   1720  HZ1 LYS   104      -2.239  14.433   7.661  1.00  0.00
ATOM   1721  HZ2 LYS   104      -2.233  14.543   5.973  1.00  0.00
ATOM   1722  HZ3 LYS   104      -0.793  14.236   6.806  1.00  0.00
ATOM   1723  C   LYS   104       1.860   8.497   7.941  1.00  0.00
ATOM   1724  O   LYS   104       2.995   8.903   8.184  1.00  0.00
ATOM   1725  N   PHE   105       1.460   7.259   8.213  1.00  0.00
ATOM   1726  HN  PHE   105       0.540   6.997   7.997  1.00  0.00
ATOM   1727  CA  PHE   105       2.351   6.279   8.824  1.00  0.00
ATOM   1728  HA  PHE   105       2.951   6.790   9.562  1.00  0.00
ATOM   1729  CB  PHE   105       1.536   5.184   9.515  1.00  0.00
ATOM   1730  HB1 PHE   105       2.007   4.228   9.338  1.00  0.00
ATOM   1731  HB2 PHE   105       0.540   5.171   9.097  1.00  0.00
ATOM   1732  CG  PHE   105       1.411   5.369  11.001  1.00  0.00
ATOM   1733  CD1 PHE   105       0.531   6.294  11.524  1.00  0.00
ATOM   1734  HD1 PHE   105      -0.083   6.867  10.853  1.00  0.00
ATOM   1735  CD2 PHE   105       2.177   4.614  11.874  1.00  0.00
ATOM   1736  HD2 PHE   105       2.872   3.889  11.478  1.00  0.00
ATOM   1737  CE1 PHE   105       0.400   6.465  12.890  1.00  0.00
ATOM   1738  HE1 PHE   105      -0.296   7.190  13.285  1.00  0.00
ATOM   1739  CE2 PHE   105       2.061   4.780  13.241  1.00  0.00
ATOM   1740  HE2 PHE   105       2.665   4.186  13.911  1.00  0.00
ATOM   1741  CZ  PHE   105       1.172   5.707  13.750  1.00  0.00
ATOM   1742  HZ  PHE   105       1.079   5.838  14.818  1.00  0.00
ATOM   1743  C   PHE   105       3.279   5.655   7.785  1.00  0.00
ATOM   1744  O   PHE   105       4.491   5.871   7.808  1.00  0.00
ATOM   1745  N   PHE   106       2.702   4.870   6.882  1.00  0.00
ATOM   1746  HN  PHE   106       1.732   4.732   6.922  1.00  0.00
ATOM   1747  CA  PHE   106       3.470   4.199   5.841  1.00  0.00
ATOM   1748  HA  PHE   106       4.078   3.441   6.316  1.00  0.00
ATOM   1749  CB  PHE   106       2.532   3.526   4.839  1.00  0.00
ATOM   1750  HB1 PHE   106       1.861   2.844   5.366  1.00  0.00
ATOM   1751  HB2 PHE   106       1.937   4.281   4.351  1.00  0.00
ATOM   1752  CG  PHE   106       3.254   2.755   3.777  1.00  0.00
ATOM   1753  CD1 PHE   106       3.931   1.590   4.091  1.00  0.00
ATOM   1754  HD1 PHE   106       3.928   1.235   5.109  1.00  0.00
ATOM   1755  CD2 PHE   106       3.267   3.202   2.469  1.00  0.00
ATOM   1756  HD2 PHE   106       2.743   4.111   2.214  1.00  0.00
ATOM   1757  CE1 PHE   106       4.601   0.679   3.118  1.00  0.00
ATOM   1758  HE1 PHE   106       5.122  -0.029   3.376  1.00  0.00
ATOM   1759  CE2 PHE   106       3.941   2.500   1.491  1.00  0.00
ATOM   1760  HE2 PHE   106       3.935   2.853   0.471  1.00  0.00
ATOM   1761  CZ  PHE   106       4.605   1.334   1.814  1.00  0.00
ATOM   1762  HZ  PHE   106       5.125   0.780   1.050  1.00  0.00
ATOM   1763  C   PHE   106       4.388   5.173   5.110  1.00  0.00
ATOM   1764  O   PHE   106       5.610   5.033   5.148  1.00  0.00
ATOM   1765  N   PHE   107       3.795   6.155   4.434  1.00  0.00
ATOM   1766  HN  PHE   107       2.814   6.212   4.432  1.00  0.00
ATOM   1767  CA  PHE   107       4.575   7.140   3.686  1.00  0.00
ATOM   1768  HA  PHE   107       5.076   6.616   2.885  1.00  0.00
ATOM   1769  CB  PHE   107       3.662   8.212   3.077  1.00  0.00
ATOM   1770  HB1 PHE   107       2.932   8.510   3.811  1.00  0.00
ATOM   1771  HB2 PHE   107       4.263   9.070   2.810  1.00  0.00
ATOM   1772  CG  PHE   107       2.918   7.770   1.838  1.00  0.00
ATOM   1773  CD1 PHE   107       3.038   6.475   1.348  1.00  0.00
ATOM   1774  HD1 PHE   107       3.674   5.771   1.863  1.00  0.00
ATOM   1775  CD2 PHE   107       2.098   8.660   1.160  1.00  0.00
ATOM   1776  HD2 PHE   107       1.995   9.670   1.528  1.00  0.00
ATOM   1777  CE1 PHE   107       2.356   6.080   0.214  1.00  0.00
ATOM   1778  HE1 PHE   107       2.460   5.069  -0.154  1.00  0.00
ATOM   1779  CE2 PHE   107       1.413   8.268   0.025  1.00  0.00
ATOM   1780  HE2 PHE   107       0.777   8.972  -0.492  1.00  0.00
ATOM   1781  CZ  PHE   107       1.542   6.977  -0.449  1.00  0.00
ATOM   1782  HZ  PHE   107       1.007   6.669  -1.336  1.00  0.00
ATOM   1783  C   PHE   107       5.636   7.787   4.571  1.00  0.00
ATOM   1784  O   PHE   107       6.638   8.301   4.075  1.00  0.00
ATOM   1785  N   SER   108       5.411   7.766   5.883  1.00  0.00
ATOM   1786  HN  SER   108       4.619   7.305   6.227  1.00  0.00
ATOM   1787  CA  SER   108       6.391   8.287   6.826  1.00  0.00
ATOM   1788  HA  SER   108       6.835   9.173   6.400  1.00  0.00
ATOM   1789  CB  SER   108       5.730   8.643   8.157  1.00  0.00
ATOM   1790  HB1 SER   108       6.468   8.597   8.942  1.00  0.00
ATOM   1791  HB2 SER   108       4.940   7.938   8.364  1.00  0.00
ATOM   1792  OG  SER   108       5.181   9.949   8.121  1.00  0.00
ATOM   1793  HG  SER   108       4.501   9.993   7.445  1.00  0.00
ATOM   1794  C   SER   108       7.471   7.243   7.042  1.00  0.00
ATOM   1795  O   SER   108       8.647   7.561   7.216  1.00  0.00
ATOM   1796  N   LYS   109       7.049   5.986   6.994  1.00  0.00
ATOM   1797  HN  LYS   109       6.100   5.811   6.828  1.00  0.00
ATOM   1798  CA  LYS   109       7.953   4.860   7.124  1.00  0.00
ATOM   1799  HA  LYS   109       8.620   5.053   7.951  1.00  0.00
ATOM   1800  CB  LYS   109       7.149   3.591   7.401  1.00  0.00
ATOM   1801  HB1 LYS   109       6.255   3.607   6.795  1.00  0.00
ATOM   1802  HB2 LYS   109       7.741   2.737   7.126  1.00  0.00
ATOM   1803  CG  LYS   109       6.734   3.440   8.856  1.00  0.00
ATOM   1804  HG1 LYS   109       5.820   2.866   8.902  1.00  0.00
ATOM   1805  HG2 LYS   109       6.566   4.421   9.276  1.00  0.00
ATOM   1806  CD  LYS   109       7.802   2.732   9.670  1.00  0.00
ATOM   1807  HD1 LYS   109       8.751   3.219   9.500  1.00  0.00
ATOM   1808  HD2 LYS   109       7.644   2.794  10.717  1.00  0.00
ATOM   1809  CE  LYS   109       7.919   1.269   9.276  1.00  0.00
ATOM   1810  HE1 LYS   109       6.930   0.835   9.256  1.00  0.00
ATOM   1811  HE2 LYS   109       8.359   1.209   8.292  1.00  0.00
ATOM   1812  NZ  LYS   109       8.763   0.502  10.233  1.00  0.00
ATOM   1813  HZ1 LYS   109       8.800  -0.499   9.955  1.00  0.00
ATOM   1814  HZ2 LYS   109       8.368   0.570  11.192  1.00  0.00
ATOM   1815  HZ3 LYS   109       9.731   0.883  10.241  1.00  0.00
ATOM   1816  C   LYS   109       8.769   4.700   5.846  1.00  0.00
ATOM   1817  O   LYS   109       9.944   4.348   5.882  1.00  0.00
ATOM   1818  N   ILE   110       8.127   4.989   4.717  1.00  0.00
ATOM   1819  HN  ILE   110       7.193   5.283   4.765  1.00  0.00
ATOM   1820  CA  ILE   110       8.780   4.928   3.416  1.00  0.00
ATOM   1821  HA  ILE   110       8.993   3.891   3.187  1.00  0.00
ATOM   1822  CB  ILE   110       7.850   5.488   2.313  1.00  0.00
ATOM   1823  HB  ILE   110       7.508   6.464   2.626  1.00  0.00
ATOM   1824  CG1 ILE   110       6.640   4.570   2.129  1.00  0.00
ATOM   1825 HG11 ILE   110       5.898   5.077   1.532  1.00  0.00
ATOM   1826 HG12 ILE   110       6.221   4.342   3.093  1.00  0.00
ATOM   1827  CG2 ILE   110       8.593   5.651   0.996  1.00  0.00
ATOM   1828 HG21 ILE   110       8.729   6.702   0.786  1.00  0.00
ATOM   1829 HG22 ILE   110       8.022   5.196   0.201  1.00  0.00
ATOM   1830 HG23 ILE   110       9.556   5.169   1.070  1.00  0.00
ATOM   1831  CD1 ILE   110       6.973   3.260   1.449  1.00  0.00
ATOM   1832 HD11 ILE   110       6.748   2.442   2.117  1.00  0.00
ATOM   1833 HD12 ILE   110       8.023   3.242   1.201  1.00  0.00
ATOM   1834 HD13 ILE   110       6.388   3.162   0.548  1.00  0.00
ATOM   1835  C   ILE   110      10.088   5.717   3.438  1.00  0.00
ATOM   1836  O   ILE   110      11.139   5.225   3.008  1.00  0.00
ATOM   1837  N   LYS   111      10.018   6.946   3.946  1.00  0.00
ATOM   1838  HN  LYS   111       9.152   7.278   4.263  1.00  0.00
ATOM   1839  CA  LYS   111      11.184   7.828   4.017  1.00  0.00
ATOM   1840  HA  LYS   111      11.336   8.250   3.035  1.00  0.00
ATOM   1841  CB  LYS   111      10.921   8.963   5.009  1.00  0.00
ATOM   1842  HB1 LYS   111      11.572   8.840   5.861  1.00  0.00
ATOM   1843  HB2 LYS   111       9.894   8.907   5.340  1.00  0.00
ATOM   1844  CG  LYS   111      11.156  10.346   4.425  1.00  0.00
ATOM   1845  HG1 LYS   111      11.692  10.245   3.493  1.00  0.00
ATOM   1846  HG2 LYS   111      11.746  10.925   5.121  1.00  0.00
ATOM   1847  CD  LYS   111       9.847  11.073   4.164  1.00  0.00
ATOM   1848  HD1 LYS   111      10.065  12.076   3.827  1.00  0.00
ATOM   1849  HD2 LYS   111       9.280  11.114   5.083  1.00  0.00
ATOM   1850  CE  LYS   111       9.018  10.367   3.104  1.00  0.00
ATOM   1851  HE1 LYS   111       8.683   9.419   3.499  1.00  0.00
ATOM   1852  HE2 LYS   111       9.636  10.195   2.235  1.00  0.00
ATOM   1853  NZ  LYS   111       7.830  11.169   2.702  1.00  0.00
ATOM   1854  HZ1 LYS   111       7.360  11.560   3.543  1.00  0.00
ATOM   1855  HZ2 LYS   111       7.151  10.571   2.187  1.00  0.00
ATOM   1856  HZ3 LYS   111       8.121  11.954   2.084  1.00  0.00
ATOM   1857  C   LYS   111      12.448   7.070   4.425  1.00  0.00
ATOM   1858  O   LYS   111      13.491   7.199   3.785  1.00  0.00
ATOM   1859  N   GLU   112      12.347   6.285   5.491  1.00  0.00
ATOM   1860  HN  GLU   112      11.489   6.225   5.962  1.00  0.00
ATOM   1861  CA  GLU   112      13.485   5.516   5.983  1.00  0.00
ATOM   1862  HA  GLU   112      14.297   6.205   6.161  1.00  0.00
ATOM   1863  CB  GLU   112      13.126   4.819   7.296  1.00  0.00
ATOM   1864  HB1 GLU   112      12.159   4.350   7.189  1.00  0.00
ATOM   1865  HB2 GLU   112      13.864   4.058   7.500  1.00  0.00
ATOM   1866  CG  GLU   112      13.070   5.760   8.489  1.00  0.00
ATOM   1867  HG1 GLU   112      12.440   5.320   9.249  1.00  0.00
ATOM   1868  HG2 GLU   112      12.644   6.700   8.169  1.00  0.00
ATOM   1869  CD  GLU   112      14.437   6.026   9.087  1.00  0.00
ATOM   1870  OE1 GLU   112      14.842   5.277  10.001  1.00  0.00
ATOM   1871  OE2 GLU   112      15.103   6.984   8.641  1.00  0.00
ATOM   1872  C   GLU   112      13.934   4.484   4.954  1.00  0.00
ATOM   1873  O   GLU   112      15.128   4.220   4.798  1.00  0.00
ATOM   1874  N   ALA   113      12.970   3.892   4.257  1.00  0.00
ATOM   1875  HN  ALA   113      12.037   4.136   4.430  1.00  0.00
ATOM   1876  CA  ALA   113      13.263   2.883   3.245  1.00  0.00
ATOM   1877  HA  ALA   113      14.151   2.356   3.550  1.00  0.00
ATOM   1878  CB  ALA   113      12.128   1.872   3.167  1.00  0.00
ATOM   1879  HB1 ALA   113      11.209   2.380   2.915  1.00  0.00
ATOM   1880  HB2 ALA   113      12.016   1.381   4.123  1.00  0.00
ATOM   1881  HB3 ALA   113      12.353   1.136   2.409  1.00  0.00
ATOM   1882  C   ALA   113      13.513   3.512   1.873  1.00  0.00
ATOM   1883  O   ALA   113      13.917   2.823   0.936  1.00  0.00
ATOM   1884  N   GLY   114      13.276   4.818   1.753  1.00  0.00
ATOM   1885  HN  GLY   114      12.946   5.324   2.523  1.00  0.00
ATOM   1886  CA  GLY   114      13.468   5.488   0.480  1.00  0.00
ATOM   1887  HA1 GLY   114      14.518   5.464   0.226  1.00  0.00
ATOM   1888  HA2 GLY   114      13.152   6.516   0.573  1.00  0.00
ATOM   1889  C   GLY   114      12.679   4.830  -0.634  1.00  0.00
ATOM   1890  O   GLY   114      13.227   4.056  -1.417  1.00  0.00
ATOM   1891  N   LEU   115      11.383   5.123  -0.690  1.00  0.00
ATOM   1892  HN  LEU   115      11.006   5.743  -0.033  1.00  0.00
ATOM   1893  CA  LEU   115      10.508   4.534  -1.697  1.00  0.00
ATOM   1894  HA  LEU   115      11.123   4.180  -2.510  1.00  0.00
ATOM   1895  CB  LEU   115       9.724   3.363  -1.104  1.00  0.00
ATOM   1896  HB1 LEU   115       9.340   3.668  -0.144  1.00  0.00
ATOM   1897  HB2 LEU   115       8.890   3.167  -1.754  1.00  0.00
ATOM   1898  CG  LEU   115      10.497   2.058  -0.907  1.00  0.00
ATOM   1899  HG  LEU   115       9.793   1.246  -0.833  1.00  0.00
ATOM   1900  CD1 LEU   115      11.280   2.102   0.391  1.00  0.00
ATOM   1901 HD11 LEU   115      10.719   1.597   1.166  1.00  0.00
ATOM   1902 HD12 LEU   115      11.440   3.130   0.674  1.00  0.00
ATOM   1903 HD13 LEU   115      12.231   1.611   0.255  1.00  0.00
ATOM   1904  CD2 LEU   115      11.414   1.774  -2.087  1.00  0.00
ATOM   1905 HD21 LEU   115      11.066   2.313  -2.953  1.00  0.00
ATOM   1906 HD22 LEU   115      11.409   0.715  -2.298  1.00  0.00
ATOM   1907 HD23 LEU   115      12.418   2.086  -1.446  1.00  0.00
ATOM   1908  C   LEU   115       9.509   5.550  -2.237  1.00  0.00
ATOM   1909  O   LEU   115       9.388   6.653  -1.709  1.00  0.00
ATOM   1910  N   ILE   116       8.752   5.124  -3.252  1.00  0.00
ATOM   1911  HN  ILE   116       8.896   4.217  -3.594  1.00  0.00
ATOM   1912  CA  ILE   116       7.707   5.945  -3.865  1.00  0.00
ATOM   1913  HA  ILE   116       7.395   5.441  -4.768  1.00  0.00
ATOM   1914  CB  ILE   116       6.469   6.061  -2.949  1.00  0.00
ATOM   1915  HB  ILE   116       6.730   6.669  -2.097  1.00  0.00
ATOM   1916  CG1 ILE   116       6.037   4.676  -2.458  1.00  0.00
ATOM   1917 HG11 ILE   116       5.298   4.265  -3.135  1.00  0.00
ATOM   1918 HG12 ILE   116       6.898   4.024  -2.435  1.00  0.00
ATOM   1919  CG2 ILE   116       5.326   6.743  -3.681  1.00  0.00
ATOM   1920 HG21 ILE   116       5.006   7.609  -3.121  1.00  0.00
ATOM   1921 HG22 ILE   116       4.502   6.052  -3.779  1.00  0.00
ATOM   1922 HG23 ILE   116       5.659   7.050  -4.661  1.00  0.00
ATOM   1923  CD1 ILE   116       5.433   4.694  -1.073  1.00  0.00
ATOM   1924 HD11 ILE   116       6.172   5.032  -0.363  1.00  0.00
ATOM   1925 HD12 ILE   116       5.110   3.698  -0.809  1.00  0.00
ATOM   1926 HD13 ILE   116       4.586   5.363  -1.057  1.00  0.00
ATOM   1927  C   ILE   116       8.213   7.340  -4.246  1.00  0.00
ATOM   1928  O   ILE   116       8.498   7.601  -5.415  1.00  0.00
ATOM   1929  N   ASP   117       8.305   8.240  -3.268  1.00  0.00
ATOM   1930  HN  ASP   117       8.072   7.979  -2.355  1.00  0.00
ATOM   1931  CA  ASP   117       8.776   9.600  -3.515  1.00  0.00
ATOM   1932  HA  ASP   117       8.982  10.054  -2.558  1.00  0.00
ATOM   1933  CB  ASP   117      10.063   9.583  -4.345  1.00  0.00
ATOM   1934  HB1 ASP   117       9.902  10.133  -5.260  1.00  0.00
ATOM   1935  HB2 ASP   117      10.317   8.560  -4.583  1.00  0.00
ATOM   1936  CG  ASP   117      11.233  10.208  -3.610  1.00  0.00
ATOM   1937  OD1 ASP   117      11.577  11.368  -3.920  1.00  0.00
ATOM   1938  OD2 ASP   117      11.804   9.538  -2.724  1.00  0.00
ATOM   1939  C   ASP   117       7.708  10.424  -4.226  1.00  0.00
ATOM   1940  O   ASP   117       8.020  11.293  -5.041  1.00  0.00
ATOM   1941  N   LYS   118       6.448  10.150  -3.906  1.00  0.00
ATOM   1942  HN  LYS   118       6.264   9.447  -3.267  1.00  0.00
ATOM   1943  CA  LYS   118       5.332  10.869  -4.508  1.00  0.00
ATOM   1944  HA  LYS   118       5.635  11.184  -5.496  1.00  0.00
ATOM   1945  CB  LYS   118       4.114   9.952  -4.628  1.00  0.00
ATOM   1946  HB1 LYS   118       3.696   9.798  -3.644  1.00  0.00
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ATOM   1947  HB2 LYS   118       4.432   9.001  -5.028  1.00  0.00
ATOM   1948  CG  LYS   118       3.021  10.506  -5.527  1.00  0.00
ATOM   1949  HG1 LYS   118       3.175  10.140  -6.531  1.00  0.00
ATOM   1950  HG2 LYS   118       3.077  11.585  -5.522  1.00  0.00
ATOM   1951  CD  LYS   118       1.642  10.081  -5.053  1.00  0.00
ATOM   1952  HD1 LYS   118       1.422   9.100  -5.449  1.00  0.00
ATOM   1953  HD2 LYS   118       1.637  10.044  -3.974  1.00  0.00
ATOM   1954  CE  LYS   118       0.569  11.052  -5.518  1.00  0.00
ATOM   1955  HE1 LYS   118      -0.025  11.347  -4.666  1.00  0.00
ATOM   1956  HE2 LYS   118       1.048  11.922  -5.942  1.00  0.00
ATOM   1957  NZ  LYS   118      -0.324  10.443  -6.543  1.00  0.00
ATOM   1958  HZ1 LYS   118      -0.736   9.558  -6.180  1.00  0.00
ATOM   1959  HZ2 LYS   118       0.214  10.234  -7.408  1.00  0.00
ATOM   1960  HZ3 LYS   118      -1.097  11.099  -6.778  1.00  0.00
ATOM   1961  C   LYS   118       4.974  12.103  -3.687  1.00  0.00
ATOM   1962  OT1 LYS   118       4.769  13.177  -4.291  1.00  0.00
ATOM   1963  OT2 LYS   118       4.901  11.986  -2.445  1.00  0.00
END
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Table 6

Atomic Structure Coordinates of the P/CAF Bromodomain/Acetyl-Histamine Complex

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REMARK
FILENAME="/bloch2/chris/COMPLEX_XPLOR_ARIA7/structures/it0/complex_03."REMARK
initial random number seed: 5.960359E+10REMARK
-------------------------------------------------------------REMARK
overall,bonds,angles,improper,vdw,noe,cdihREMARK energies: 154.107, 9.85626,
72.1621, 0, 22.2303, 36.0151, 0.204524REMARK
-------------------------------------------------------------REMARK
bonds,angles,impropers,noe,cdihREMARK rms-dev.: 2.214961E-
03,0.361077,52.7899,1.40651E-02,0.249335REMARK
-------------------------------------------------------------REMARK
noe,  cdihREMARK violations.: 2, 0REMARK
-------------------------------------------------------------REMARK DATE:05-
Dec-98  15:11:47       created by user:ATOM      1  CA  ACE   200      -14.038
2.661  -4.708  1.00  0.00      AcH ATOM      2  HA1 ACE   200      -14.603
1.912  -4.558  1.00  0.00      AcH ATOM      3  HA2 ACE   200      -13.320
2.304  -5.428  1.00  0.00      AcH ATOM      4  HA3 ACE   200      -14.491
3.572  -5.067  1.00  0.00      AcH ATOM      5  C   ACE   200      -13.332
2.936  -3.376  1.00  0.00      AcH ATOM      6  O   ACE   200      -12.365
2.238  -3.012  1.00  0.00      AcH ATOM      7  N   HIM   201      -13.773
3.967  -2.663  1.00  0.00      AcH ATOM      8  HN  HIM   201      -13.586
4.875  -2.982  1.00  0.00      AcH ATOM      9  CA  HIM   201      -14.521
3.827  -1.417  1.00  0.00      AcH ATOM     10  HA1 HIM   201      -13.833
3.589  -0.620  1.00  0.00      AcH ATOM     11  HA2 HIM   201      -15.236
3.025  -1.526  1.00  0.00      AcH ATOM     12  CB  HIM   201      -15.268
5.100  -1.055  1.00  0.00      AcH ATOM     13  HB1 HIM   201      -14.591
5.940  -1.107  1.00  0.00      AcH ATOM     14  HB2 HIM   201      -15.669
5.009  -0.056  1.00  0.00      AcH ATOM     15  CG  HIM   201      -16.397
5.329  -2.010  1.00  0.00      AcH ATOM     16  ND1 HIM   201      -17.392
6.259  -1.793  1.00  0.00      AcH ATOM     17  HD1 HIM   201      -17.421
4.906  -1.057  1.00  0.00      AcH ATOM     18  CD2 HIM   201      -16.680
4.756  -3.204  1.00  0.00      AcH ATOM     19  HD2 HIM   201      -16.026
4.116  -3.779  1.00  0.00      AcH ATOM     20  CE1 HIM   201      -18.316
6.135  -2.729  1.00  0.00      AcH ATOM     21  HE1 HIM   201      -19.220
6.722  -2.806  1.00  0.00      AcH ATOM     22  NE2 HIM   201      -17.912
5.221  -3.592  1.00  0.00      AcH ATOM     23  CA  GLY     1       27.272
16.667  -0.366  1.00  0.00      BrD ATOM     24  HA1 GLY     1       28.103
16.198  -0.871  1.00  0.00      BrD ATOM     25  HA2 GLY     1       26.478
15.945  -0.255  1.00  0.00      BrD ATOM     26  C   GLY     1       27.724
17.114   1.011  1.00  0.00      BrD ATOM     27  O   GLY     1       28.713
17.836   1.144  1.00  0.00      BrD ATOM     28  N   GLY     1       26.780
17.800  -1.198  1.00  0.00      BrD ATOM     29  HT1 GLY     1       25.768
17.963  -1.018  1.00  0.00      BrD ATOM     30  HT2 GLY     1       26.911
17.584  -2.207  1.00  0.00      BrD ATOM     31  HT3 GLY     1       27.307
16.667  -0.970  1.00  0.00      BrD ATOM     32  N   SER     2       26.999
16.682   2.037  1.00  0.00      BrD ATOM     33  HN  SER     2       26.222
16.110   1.866  1.00  0.00      BrD ATOM     34  CA  SER     2       27.328
17.043   3.411  1.00  0.00      BrD ATOM     35  HA  SER     2       28.283
17.546   3.401  1.00  0.00      BrD ATOM     36  CB  SER     2       26.269
17.992   3.975  1.00  0.00      BrD ATOM     37  HB1 SER     2       26.705
18.588   4.762  1.00  0.00      BrD ATOM     38  HB2 SER     2       25.448
17.414   4.174  1.00  0.00      BrD ATOM     39  OG  SER     2       25.771
18.857   2.969  1.00  0.00      BrD ATOM     40  HG  SER     2       26.478
19.429   2.660  1.00  0.00      BrD ATOM     41  C   SER     2       27.435
15.801   4.290  1.00  0.00      BrD ATOM     42  O   SER     2       26.900
14.744   3.956  1.00  0.00      BrD ATOM     43  N   HIS     3       28.131
15.936   5.415  1.00  0.00      BrD ATOM     44  HN  HIS     3       28.534
16.803   5.627  1.00  0.00      BrD ATOM     45  CA  HIS     3       28.308
14.824   6.342  1.00  0.00      BrD ATOM     46  HA  HIS     3       28.652
13.972   5.775  1.00  0.00      BrD ATOM     47  CB  HIS     3       29.356
15.176   7.399  1.00  0.00      BrD ATOM     48  HB1 HIS     3       29.337
14.428   8.178  1.00  0.00      BrD ATOM     49  HB2 HIS     3       30.333
15.184   6.939  1.00  0.00      BrD ATOM     50  CG  HIS     3       29.137
16.512   8.039  1.00  0.00      BrD ATOM     51  ND1 HIS     3       28.235
16.718   9.062  1.00  0.00      BrD ATOM     52  HD1 HIS     3       27.659
16.035   9.465  1.00  0.00      BrD ATOM     53  CD2 HIS     3       29.710
17.715   7.796  1.00  0.00      BrD ATOM     54  HD2 HIS     3       30.468
17.927   7.055  1.00  0.00      BrD ATOM     55  CE1 HIS     3       28.262
17.991   9.420  1.00  0.00      BrD ATOM     56  HE1 HIS     3       27.661
18.442  10.196  1.00  0.00      BrD ATOM     57  NE2 HIS     3       29.148
18.615   8.668  1.00  0.00      BrD ATOM     58  HE2 HIS     3       29.368
19.568   8.725  1.00  0.00      BrD ATOM     59  C   HIS     3       26.991
14.463   7.020  1.00  0.00      BrD ATOM     60  O   HIS     3       26.660
14.998   8.078  1.00  0.00      BrD ATOM     61  N   MET     4       26.245
13.551   6.405  1.00  0.00      BrD ATOM     62  HN  MET     4       26.563
13.161   5.565  1.00  0.00      BrD ATOM     63  CA  MET     4       24.964
13.119   6.951  1.00  0.00      BrD ATOM     64  HA  MET     4       25.136
12.767   7.958  1.00  0.00      BrD ATOM     65  CB  MET     4       23.985
14.294   6.994  1.00  0.00      BrD ATOM     66  HB1 MET     4       24.445
15.111   7.531  1.00  0.00      BrD ATOM     67  HB2 MET     4       23.776
14.612   5.984  1.00  0.00      BrD ATOM     68  CG  MET     4       22.665
13.962   7.672  1.00  0.00      BrD ATOM     69  HG1 MET     4       22.754
14.176   8.727  1.00  0.00      BrD ATOM     70  HG2 MET     4       22.461
12.911   7.535  1.00  0.00      BrD ATOM     71  SD  MET     4       21.283
14.909   7.006  1.00  0.00      BrD ATOM     72  CE  MET     4       22.027
16.531   6.842  1.00  0.00      BrD ATOM     73  HE1 MET     4       22.811
16.643   7.576  1.00  0.00      BrD ATOM     74  HE2 MET     4       21.274
17.289   7.000  1.00  0.00      BrD ATOM     75  HE3 MET     4       22.443
16.638   5.851  1.00  0.00      BrD ATOM     76  C   MET     4       24.376
11.977   6.126  1.00  0.00      BrD ATOM     77  O   MET     4       24.580
11.906   4.914  1.00  0.00      BrD ATOM     78  N   SER     5       23.650
11.084   6.792  1.00  0.00      BrD ATOM     79  HN  SER     5       23.528
11.194   7.758  1.00  0.00      BrD ATOM     80  CA  SER     5       23.040
9.939   6.125  1.00  0.00      BrD ATOM     81  HA  SER     5       23.836
9.303   5.767  1.00  0.00      BrD ATOM     82  CB  SER     5       22.177
9.148   7.111  1.00  0.00      BrD ATOM     83  HB1 SER     5       21.179
9.560   7.123  1.00  0.00      BrD ATOM     84  HB2 SER     5       22.136
8.114   6.801  1.00  0.00      BrD ATOM     85  OG  SER     5       22.712
9.210   8.421  1.00  0.00      BrD ATOM     86  HG  SER     5       23.243
8.428   8.588  1.00  0.00      BrD ATOM     87  C   SER     5       22.194
10.380   4.934  1.00  0.00      BrD ATOM     88  O   SER     5       21.748
11.525   4.867  1.00  0.00      BrD ATOM     89  N   LYS     6       21.973
9.460   3.999  1.00  0.00      BrD ATOM     90  HN  LYS     6       22.355
8.565   4.110  1.00  0.00      BrD ATOM     91  CA  LYS     6       21.180
9.753   2.811  1.00  0.00      BrD ATOM     92  HA  LYS     6       20.720
10.720   2.950  1.00  0.00      BrD ATOM     93  CB  LYS     6       22.078
9.801   1.573  1.00  0.00      BrD ATOM     94  HB1 LYS     6       21.474
10.056   0.714  1.00  0.00      BrD ATOM     95  HB2 LYS     6       22.512
8.824   1.418  1.00  0.00      BrD ATOM     96  CG  LYS     6       23.208
10.813   1.677  1.00  0.00      BrD ATOM     97  HG1 LYS     6       23.164
11.290   2.645  1.00  0.00      BrD ATOM     98  HG2 LYS     6       24.151
10.299   1.568  1.00  0.00      BrD ATOM     99  CD  LYS     6       23.100
11.879   0.598  1.00  0.00      BrD ATOM    100  HD1 LYS     6       22.401
11.546  -0.155  1.00  0.00      BrD ATOM    101  HD2 LYS     6       24.072
12.024   0.150  1.00  0.00      BrD ATOM    102  CE  LYS     6       22.618
13.203   1.168  1.00  0.00      BrD ATOM    103  HE1 LYS     6       21.595
13.088   1.494  1.00  0.00      BrD ATOM    104  HE2 LYS     6       22.666
13.953   0.393  1.00  0.00      BrD ATOM    105  NZ  LYS     6       23.448
13.645   2.322  1.00  0.00      BrD ATOM    106  HZ1 LYS     6       24.293
13.045   2.406  1.00  0.00      BrD ATOM    107  HZ2 LYS     6       22.900
13.578   3.204  1.00  0.00      BrD ATOM    108  HZ3 LYS     6       23.749
14.632   2.189  1.00  0.00      BrD ATOM    109  C   LYS     6       20.085
8.710   2.613  1.00  0.00      BrD ATOM    110  O   LYS     6       18.897
9.022   2.693  1.00  0.00      BrD ATOM    111  N   GLU     7       20.495
7.474   2.334  1.00  0.00      BrD ATOM    112  HN  GLU     7       21.457
7.295   2.280  1.00  0.00      BrD ATOM    113  CA  GLU     7       19.558
6.370   2.115  1.00  0.00      BrD ATOM    114  HA  GLU     7       20.083
5.603   1.565  1.00  0.00      BrD ATOM    115  CB  GLU     7       19.091
5.783   3.451  1.00  0.00      BrD ATOM    116  HB1 GLU     7       18.110
5.356   3.317  1.00  0.00      BrD ATOM    117  HB2 GLU     7       19.777
5.003   3.745  1.00  0.00      BrD ATOM    118  CG  GLU     7       19.014
6.799   4.579  1.00  0.00      BrD ATOM    119  HG1 GLU     7       18.377
7.614   4.271  1.00  0.00      BrD ATOM    120  HG2 GLU     7       20.007
7.173   4.780  1.00  0.00      BrD ATOM    121  CD  GLU     7       18.452
6.206   5.857  1.00  0.00      BrD ATOM    122  OE1 GLU     7       17.289
6.511   6.192  1.00  0.00      BrD ATOM    123  OE2 GLU     7       19.176
5.434   6.521  1.00  0.00      BrD ATOM    124  C   GLU     7       18.347
6.812   1.290  1.00  0.00      BrD ATOM    125  O   GLU     7       17.342
7.261   1.840  1.00  0.00      BrD ATOM    126  N   PRO     8       18.430
6.681  -0.045  1.00  0.00      BrD ATOM    127  CA  PRO     8       17.346
7.054  -0.951  1.00  0.00      BrD ATOM    128  HA  PRO     8       16.908
8.003  -0.677  1.00  0.00      BrD ATOM    129  CB  PRO     8       18.034
7.176  -2.321  1.00  0.00      BrD ATOM    130  HB1 PRO     8       17.603
6.458  -3.004  1.00  0.00      BrD ATOM    131  HB2 PRO     8       17.887
8.174  -2.708  1.00  0.00      BrD ATOM    132  CG  PRO     8       19.488
6.895  -2.087  1.00  0.00      BrD ATOM    133  HG1 PRO     8       19.876
6.286  -2.890  1.00  0.00      BrD ATOM    134  HG2 PRO     8       20.034
7.825  -2.026  1.00  0.00      BrD ATOM    135  CD  PRO     8       19.578
6.155  -0.784  1.00  0.00      BrD ATOM    136  HD1 PRO     8       20.504
6.384  -0.278  1.00  0.00      BrD ATOM    137  HD2 PRO     8       19.481
5.090  -0.943  1.00  0.00      BrD ATOM    138  C   PRO     8       16.259
5.987  -1.000  1.00  0.00      BrD ATOM    139  O   PRO     8       15.071
6.286  -0.874  1.00  0.00      BrD ATOM    140  N   ARG     9       16.680
4.740  -1.177  1.00  0.00      BrD ATOM    141  HN  ARG     9       17.640
4.570  -1.269  1.00  0.00      BrD ATOM    142  CA  ARG     9       15.754
3.617  -1.241  1.00  0.00      BrD ATOM    143  HA  ARG     9       15.272
3.529  -0.279  1.00  0.00      BrD ATOM    144  CB  ARG     9       14.692
3.864  -2.314  1.00  0.00      BrD ATOM    145  HB1 ARG     9       14.073
2.982  -2.402  1.00  0.00      BrD ATOM    146  HB2 ARG     9       14.076
4.696  -2.010  1.00  0.00      BrD ATOM    147  CG  ARG     9       15.272
4.176  -3.684  1.00  0.00      BrD ATOM    148  HG1 ARG     9       16.153
3.571  -3.837  1.00  0.00      BrD ATOM    149  HG2 ARG     9       15.519
5.221  -3.721  1.00  0.00      BrD ATOM    150  CD  ARG     9       14.274
3.882  -4.793  1.00  0.00      BrD ATOM    151  HD1 ARG     9       13.277
4.055  -4.417  1.00  0.00      BrD ATOM    152  HD2 ARG     9       14.375
2.848  -5.085  1.00  0.00      BrD ATOM    153  NE  ARG     9       14.493
4.728  -5.963  1.00  0.00      BrD ATOM    154  HE  ARG     9       14.761
4.289  -6.797  1.00  0.00      BrD ATOM    155  CZ  ARG     9       14.350
6.049  -5.955  1.00  0.00      BrD ATOM    156  NH1 ARG     9       13.988
6.672  -4.842  1.00  0.00      BrD ATOM    157 HH11 ARG     9       13.823
6.147  -4.006  1.00  0.00      BrD ATOM    158 HH12 ARG     9       13.880
7.666  -4.837  1.00  0.00      BrD ATOM    159  NH2 ARG     9       14.567
6.749  -7.059  1.00  0.00      BrD ATOM    160 HH21 ARG     9       14.458
7.744  -7.051  1.00  0.00      BrD ATOM    161 HH22 ARG     9       14.840
6.284  -7.901  1.00  0.00      BrD ATOM    162  C   ARG     9       16.500
2.320  -1.538  1.00  0.00      BrD ATOM    163  O   ARG     9       17.367
2.278  -2.410  1.00  0.00      BrD ATOM    164  N   ASP    10       16.159
1.267  -0.803  1.00  0.00      BrD ATOM    165  HN  ASP    10       15.462
1.367  -0.123  1.00  0.00      BrD ATOM    166  CA  ASP    10       16.788
0.038  -0.988  1.00  0.00      BrD ATOM    167  HA  ASP    10       17.625
0.088  -1.658  1.00  0.00      BrD ATOM    168  CB  ASP    10       17.396
0.576   0.350  1.00  0.00      BrD ATOM    169  HB1 ASP    10       18.082
0.067   0.715  1.00  0.00      BrD ATOM    170  HB2 ASP    10       17.688
1.572   0.204  1.00  0.00      BrD ATOM    171  CG  ASP    10       16.203
0.641   1.399  1.00  0.00      BrD ATOM    172  OD1 ASP    10       16.210
1.595   2.205  1.00  0.00      BrD ATOM    173  OD2 ASP    10       15.340
0.262   1.413  1.00  0.00      BrD ATOM    174  C   ASP    10       15.803
1.028  -1.606  1.00  0.00      BrD ATOM    175  O   ASP    10       14.986
1.622  -0.903  1.00  0.00      BrD ATOM    176  N   PRO    11       15.866
1.218  -2.936  1.00  0.00      BrD ATOM    177  CA  PRO    11       14.974
2.118  -3.657  1.00  0.00      BrD ATOM    178  HA  PRO    11       13.975
2.098  -3.247  1.00  0.00      BrD ATOM    179  CB  PRO    11       14.958
1.540  -5.084  1.00  0.00      BrD ATOM    180  HB1 PRO    11       13.973
1.156  -5.302  1.00  0.00      BrD ATOM    181  HB2 PRO    11       15.203
2.321  -5.789  1.00  0.00      BrD ATOM    182  CG  PRO    11       15.982
0.443  -5.113  1.00  0.00      BrD ATOM    183  HG1 PRO    11       15.467
0.516  -5.149  1.00  0.00      BrD ATOM    184  HG2 PRO    11       16.620
0.564  -5.976  1.00  0.00      BrD ATOM    185  CD  PRO    11       16.792
0.558  -3.852  1.00  0.00      BrD ATOM    186  HD1 PRO    11       17.066
0.418  -3.467  1.00  0.00      BrD ATOM    187  HD2 PRO    11       17.671
1.163  -4.018  1.00  0.00      BrD ATOM    188  C   PRO    11       15.488
3.554  -3.670  1.00  0.00      BrD ATOM    189  O   PRO    11       15.881
4.191  -4.721  1.00  0.00      BrD ATOM    190  N   ASP    12       15.049
4.061  -2.496  1.00  0.00      BrD ATOM    191  HN  ASP    12       15.780
3.506  -1.691  1.00  0.00      BrD ATOM    192  CA  ASP    12       16.361
5.421  -2.384  1.00  0.00      BrD ATOM    193  HA  ASP    12       16.155
5.927  -3.315  1.00  0.00      BrD ATOM    194  CB  ASP    12       17.873
5.399  -2.151  1.00  0.00      BrD ATOM    195  HB1 ASP    12       18.123
6.112  -1.380  1.00  0.00      BrD ATOM    196  HB2 ASP    12       18.167
4.410  -1.830  1.00  0.00      BrD ATOM    197  CG  ASP    12       18.657
5.749  -3.400  1.00  0.00      BrD ATOM    198  OD1 ASP    12       18.450
5.084  -4.437  1.00  0.00      BrD ATOM    199  OD2 ASP    12       19.478
6.687  -3.342  1.00  0.00      BrD ATOM    200  C   ASP    12       15.674
6.179  -1.253  1.00  0.00      BrD ATOM    201  O   ASP    12       15.106
7.250  -1.468  1.00  0.00      BrD ATOM    202  N   GLN    13       15.740
5.626  -0.047  1.00  0.00      BrD ATOM    203  HN  GLN    13       16.206
4.770   0.063  1.00  0.00      BrD ATOM    204  CA  GLN    13       15.122
4.258   1.113  1.00  0.00      BrD ATOM    205  HA  GLN    13       15.336
7.316   1.069  1.00  0.00      BrD ATOM    206  CB  GLN    13       15.701
5.684   2.405  1.00  0.00      BrD ATOM    207  HB1 GLN    13       16.666
5.251   2.193  1.00  0.00      BrD ATOM    208  HB2 GLN    13       15.041
4.910   2.768  1.00  0.00      BrD ATOM    209  CG  GLN    13       15.870
6.719   3.505  1.00  0.00      BrD ATOM    210  HG1 GLN    13       15.520
6.297   4.436  1.00  0.00      BrD ATOM    211  HG2 GLN    13       15.277
7.567   3.268  1.00  0.00      BrD ATOM    212  CD  GLN    13       17.313
7.150   3.683  1.00  0.00      BrD ATOM    213  OE1 GLN    13       18.036
6.611   4.520  1.00  0.00      BrD ATOM    214  NE2 GLN    13       17.739
8.128   2.892  1.00  0.00      BrD ATOM    215 HE21 GLN    13       18.668
8.427   2.985  1.00  0.00      BrD ATOM    216 HE22 GLN    13       17.108
8.512   2.248  1.00  0.00      BrD ATOM    217  C   GLN    13       13.615
6.060   1.097  1.00  0.00      BrD ATOM    218  O   GLN    13       12.859
6.950   1.478  1.00  0.00      BrD ATOM    219  N   LEU    14       13.191
4.880   0.662  1.00  0.00      BrD ATOM    220  HN  LEU    14       13.848
4.214   0.371  1.00  0.00      BrD ATOM    221  CA  LEU    14       11.774
4.558   0.595  1.00  0.00      BrD ATOM    222  HA  LEU    14       11.303
4.943   1.487  1.00  0.00      BrD ATOM    223  CB  LEU    14       11.581
3.042   0.561  1.00  0.00      BrD ATOM    224  HB1 LEU    14       12.212
2.592   1.292  1.00  0.00      BrD ATOM    225  HB2 LEU    14       10.552
2.823   0.781  1.00  0.00      BrD ATOM    226  CG  LEU    14       11.905
2.399  -0.808  1.00  0.00      BrD ATOM    227  HG  LEU    14       12.685
2.967  -1.292  1.00  0.00      BrD ATOM    228  CD1 LEU    14       12.409
0.978  -0.615  1.00  0.00      BrD ATOM    229 HD11 LEU    14       11.569
0.311  -0.497  1.00  0.00      BrD ATOM    230 HD12 LEU    14       12.986
0.682  -1.479  1.00  0.00      BrD ATOM    231 HD13 LEU    14       13.032
0.934   0.266  1.00  0.00      BrD ATOM    232  CD2 LEU    14       10.682
2.418  -1.709  1.00  0.00      BrD ATOM    233 HD21 LEU    14       10.185
1.461  -1.660  1.00  0.00      BrD ATOM    234 HD22 LEU    14       10.005
3.192  -1.383  1.00  0.00      BrD ATOM    235 HD23 LEU    14       10.989
2.612  -2.727  1.00  0.00      BrD ATOM    236  C   LEU    14       11.130
5.209  -0.623  1.00  0.00      BrD ATOM    237  O   LEU    14        9.989
5.666  -0.564  1.00  0.00      BrD ATOM    238  N   TYR    15       11.866
5.241  -1.729  1.00  0.00      BrD ATOM    239  HN  TYR    15       12.772
4.865  -1.714  1.00  0.00      BrD ATOM    240  CA  TYR    15       11.364
5.641  -2.959  1.00  0.00      BrD ATOM    241  HA  TYR    15       10.539
5.237  -3.312  1.00  0.00      BrD ATOM    242  CB  TYR    15       12.460
5.865  -4.029  1.00  0.00      BrD ATOM    243  HB1 TYR    15       13.317
6.397  -3.642  1.00  0.00      BrD ATOM    244  HB2 TYR    15       12.748
4.850  -4.259  1.00  0.00      BrD ATOM    245  CG  TYR    15       12.043
6.533  -5.323  1.00  0.00      BrD ATOM    246  CD1 TYR    15       12.993
7.047  -6.197  1.00  0.00      BrD ATOM    247  HD1 TYR    15       14.040
6.968  -5.940  1.00  0.00      BrD ATOM    248  CD2 TYR    15       10.702
6.642  -5.675  1.00  0.00      BrD ATOM    249  HD2 TYR    15        9.950
6.248  -5.008  1.00  0.00      BrD ATOM    250  CE1 TYR    15       12.620
7.684  -7.381  1.00  0.00      BrD ATOM    251  HE1 TYR    15       13.374
8.049  -8.046  1.00  0.00      BrD ATOM    252  CE2 TYR    15       10.322
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7.249  -6.857  1.00  0.00      BrD ATOM    253  HE2 TYR   15       9.275 -
7.326  -7.111  1.00  0.00      BrD ATOM    254  CZ  TYR   15      11.284 -
7.752  -7.706  1.00  0.00      BrD ATOM    255  OH  TYR   15      10.908 -
8.358  -8.883  1.00  0.00      BrD ATOM    256  HH  TYR   15      10.572 -
9.238  -8.697  1.00  0.00      BrD ATOM    257  C   TYR   15      10.859 -
7.253  -2.696  1.00  0.00      BrD ATOM    258  O   TYR   15       9.778 -
7.630  -3.146  1.00  0.00      BrD ATOM    259  N   SER   16      11.641 -
8.026  -1.950  1.00  0.00      BrD ATOM    260  HN  SER   16      12.485 -
7.666  -1.605  1.00  0.00      BrD ATOM    261  CA  SER   16      11.249 -
9.384  -1.602  1.00  0.00      BrD ATOM    262  HA  SER   16      11.148 -
9.946  -2.518  1.00  0.00      BrD ATOM    263  CB  SER   16      12.315 -
10.040  -0.722  1.00  0.00     BrD ATOM    264  HB1 SER   16      12.503 -
9.416   0.139  1.00  0.00      BrD ATOM    265  HB2 SER   16      13.227 -
10.155  -1.289  1.00  0.00     BrD ATOM    266  OG  SER   16      11.892 -
11.317  -0.276  1.00  0.00     BrD ATOM    267  HG  SER   16      12.601 -
11.952  -0.405  1.00  0.00     BrD ATOM    268  C   SER   16       9.909 -
9.370  -0.879  1.00  0.00      BrD ATOM    269  O   SER   16       9.028 -
10.162  -1.161  1.00  0.00     BrD ATOM    270  N   THR   17       9.756 -
8.420   0.038  1.00  0.00      BrD ATOM    271  HN  THR   17      10.493 -
7.796   0.207  1.00  0.00      BrD ATOM    272  CA  THR   17       8.514 -
8.269   0.785  1.00  0.00      BrD ATOM    273  HA  THR   17       8.318 -
9.200   1.296  1.00  0.00      BrD ATOM    274  CB  THR   17       8.656 -
7.146   1.820  1.00  0.00      BrD ATOM    275  HB  THR   17       9.069 -
6.275   1.333  1.00  0.00      BrD ATOM    276  OG1 THR   17       9.539 -
7.535   2.857  1.00  0.00      BrD ATOM    277  HG1 THR   17      10.426 -
7.633   2.502  1.00  0.00      BrD ATOM    278  CG2 THR   17       7.344 -
6.733   3.463  1.00  0.00      BrD ATOM    279  HG21 THR  17       6.714 -
7.600   2.589  1.00  0.00      BrD ATOM    280  HG22 THR  17       6.845 -
6.012   1.832  1.00  0.00      BrD ATOM    281  HG23 THR  17       7.565 -
6.289   3.427  1.00  0.00      BrD ATOM    282  C   THR   17       7.356 -
7.971  -0.161  1.00  0.00      BrD ATOM    283  O   THR   17       6.420 -
8.757  -0.277  1.00  0.00      BrD ATOM    284  N   LEU   18       7.438 -
6.832  -0.843  1.00  0.00      BrD ATOM    285  HN  LEU   18       8.212 -
6.247  -0.702  1.00  0.00      BrD ATOM    286  CA  LEU   18       6.396 -
6.414  -1.776  1.00  0.00      BrD ATOM    287  HA  LEU   18       5.534 -
6.122  -1.197  1.00  0.00      BrD ATOM    288  CB  LEU   18       6.871 -
5.218  -2.591  1.00  0.00      BrD ATOM    289  HB1 LEU   18       7.669 -
5.542  -3.243  1.00  0.00      BrD ATOM    290  HB2 LEU   18       6.049 -
4.869  -3.198  1.00  0.00      BrD ATOM    291  CG  LEU   18       7.377 -
4.056  -1.750  1.00  0.00      BrD ATOM    292  HG  LEU   18       8.301 -
4.350  -1.275  1.00  0.00      BrD ATOM    293  CD1 LEU   18       7.653 -
2.840  -2.622  1.00  0.00      BrD ATOM    294  HD11 LEU  18       6.966 -
2.832  -3.455  1.00  0.00      BrD ATOM    295  HD12 LEU  18       8.667 -
2.885  -2.994  1.00  0.00      BrD ATOM    296  HD13 LEU  18       7.523 -
1.941  -2.039  1.00  0.00      BrD ATOM    297  CD2 LEU   18       6.369 -
3.727  -0.658  1.00  0.00      BrD ATOM    298  HD21 LEU  18       5.417 -
4.180  -0.897  1.00  0.00      BrD ATOM    299  HD22 LEU  18       6.252 -
2.657  -0.584  1.00  0.00      BrD ATOM    300  HD23 LEU  18       6.722 -
4.117   0.284  1.00  0.00      BrD ATOM    301  C   LEU   18       5.998 -
7.542  -2.707  1.00  0.00      BrD ATOM    302  O   LEU   18       4.869 -
8.021  -2.667  1.00  0.00      BrD ATOM    303  N   LYS   19       6.926 -
7.967  -3.552  1.00  0.00      BrD ATOM    304  HN  LYS   19       7.813 -
7.550  -3.543  1.00  0.00      BrD ATOM    305  CA  LYS   19       6.648 -
9.050  -4.487  1.00  0.00      BrD ATOM    306  HA  LYS   19       5.959 -
8.673  -5.228  1.00  0.00      BrD ATOM    307  CB  LYS   19       7.935 -
9.498  -5.193  1.00  0.00      BrD ATOM    308  HB1 LYS   19       7.671 -
9.974  -6.126  1.00  0.00      BrD ATOM    309  HB2 LYS   19       8.538 -
8.625  -5.404  1.00  0.00      BrD ATOM    310  CG  LYS   19       8.785 -
10.472  -4.390  1.00  0.00     BrD ATOM    311  HG1 LYS   19       8.296 -
11.438  -4.386  1.00  0.00     BrD ATOM    312  HG2 LYS   19       8.878 -
10.106  -3.378  1.00  0.00     BrD ATOM    313  CD  LYS   19      10.172 -
10.621  -4.992  1.00  0.00     BrD ATOM    314  HD1 LYS   19      10.575 -
9.638  -5.190  1.00  0.00      BrD ATOM    315  HD2 LYS   19      10.807 -
11.137  -4.287  1.00  0.00     BrD ATOM    316  CE  LYS   19      10.133 -
11.409  -6.290  1.00  0.00     BrD ATOM    317  HE1 LYS   19       9.337 -
11.019  -6.908  1.00  0.00     BrD ATOM    318  HE2 LYS   19      11.077 -
11.288  -6.800  1.00  0.00     BrD ATOM    319  NZ  LYS   19       9.893 -
12.858  -6.050  1.00  0.00     BrD ATOM    320  HZ1 LYS   19       9.982 -
13.072  -5.036  1.00  0.00     BrD ATOM    321  HZ2 LYS   19      10.587 -
13.427  -6.576  1.00  0.00     BrD ATOM    322  HZ3 LYS   19       8.937 -
13.119  -6.366  1.00  0.00     BrD ATOM    323  C   LYS   19       5.988 -
10.223  -3.761  1.00  0.00     BrD ATOM    324  O   LYS   19       5.193 -
10.960  -4.341  1.00  0.00     BrD ATOM    325  N   SER   20       6.299 -
10.359  -2.474  1.00  0.00     BrD ATOM    326  HN  SER   20       6.925 -
9.721  -2.061  1.00  0.00      BrD ATOM    327  CA  SER   20       5.722 -
11.425  -1.661  1.00  0.00     BrD ATOM    328  HA  SER   20       5.660 -
12.306  -2.277  1.00  0.00     BrD ATOM    329  CB  SER   20       6.608 -
11.725  -0.449  1.00  0.00     BrD ATOM    330  HB1 SER   20       7.086 -
10.815  -0.120  1.00  0.00     BrD ATOM    331  HB2 SER   20       5.999 -
12.121   0.350  1.00  0.00     BrD ATOM    332  OG  SER   20       7.610 -
12.674  -0.772  1.00  0.00     BrD ATOM    333  HG  SER   20       7.218 -
13.396  -1.269  1.00  0.00     BrD ATOM    334  C   SER   20       4.316 -
11.056  -1.207  1.00  0.00     BrD ATOM    335  O   SER   20       3.334 -
11.659  -1.642  1.00  0.00     BrD ATOM    336  N   ILE   21       4.218 -
10.045  -0.349  1.00  0.00     BrD ATOM    337  HN  ILE   21       5.031 -
9.592  -0.044  1.00  0.00      BrD ATOM    338  CA  ILE   21       2.919 -
9.583   0.129  1.00  0.00      BrD ATOM    339  HA  ILE   21       2.508 -
10.348   0.771  1.00  0.00     BrD ATOM    340  CB  ILE   21       3.036 -
8.280   0.945  1.00  0.00      BrD ATOM    341  HB  ILE   21       2.050 -
7.850   1.036  1.00  0.00      BrD ATOM    342  CG1 ILE   21       3.956 -
7.280   0.240  1.00  0.00      BrD ATOM    343  HG11 ILE  21       4.639 -
6.458   0.962  1.00  0.00      BrD ATOM    344  HG12 ILE  21       4.519 -
7.792  -0.821  1.00  0.00      BrD ATOM    345  CG2 ILE   21       3.549 -
8.579   2.346  1.00  0.00      BrD ATOM    346  HG21 ILE  21       4.618 -
8.431   2.377  1.00  0.00      BrD ATOM    347  HG22 ILE  21       3.319 -
9.603   2.603  1.00  0.00      BrD ATOM    348  HG23 ILE  21       3.073 -
7.915   3.053  1.00  0.00      BrD ATOM    349  CD1 ILE   21       3.222 -
6.140  -0.427  1.00  0.00      BrD ATOM    350  HD11 ILE  21       3.805 -
5.235  -0.338  1.00  0.00      BrD ATOM    351  HD12 ILE  21       2.264 -
6.000   0.051  1.00  0.00      BrD ATOM    352  HD13 ILE  21       3.075 -
6.371  -1.472  1.00  0.00      BrD ATOM    353  C   ILE   21       1.969 -
9.361  -1.044  1.00  0.00      BrD ATOM    354  O   ILE   21       0.869 -
9.901  -1.074  1.00  0.00      BrD ATOM    355  N   LEU   22       2.433 -
8.608  -2.034  1.00  0.00      BrD ATOM    356  HN  LEU   22       3.325 -
8.224  -1.957  1.00  0.00      BrD ATOM    357  CA  LEU   22       1.648 -
8.337  -3.229  1.00  0.00      BrD ATOM    358  HA  LEU   22       0.757 -
7.807  -2.929  1.00  0.00      BrD ATOM    359  CB  LEU   22       2.451 -
7.465  -4.197  1.00  0.00      BrD ATOM    360  HB1 LEU   22       3.352 -
7.996  -4.462  1.00  0.00      BrD ATOM    361  HB2 LEU   22       2.728 -
6.556  -3.683  1.00  0.00      BrD ATOM    362  CG  LEU   22       1.722 -
7.084  -5.486  1.00  0.00      BrD ATOM    363  HG  LEU   22       1.378 -
7.982  -5.977  1.00  0.00      BrD ATOM    364  CD1 LEU   22       2.665 -
6.362  -6.437  1.00  0.00      BrD ATOM    365  HD11 LEU  22       2.220 -
6.314  -7.419  1.00  0.00      BrD ATOM    366  HD12 LEU  22       3.601 -
6.898  -6.492  1.00  0.00      BrD ATOM    367  HD13 LEU  22       2.845 -
5.361  -6.074  1.00  0.00      BrD ATOM    368  CD2 LEU   22       0.507 -
6.222  -5.178  1.00  0.00      BrD ATOM    369  HD21 LEU  22       0.127 -
6.472  -4.199  1.00  0.00      BrD ATOM    370  HD22 LEU  22      -0.259 -
6.401  -5.918  1.00  0.00      BrD ATOM    371  HD23 LEU  22       0.790 -
5.180  -5.199  1.00  0.00      BrD ATOM    372  C   LEU   22       1.243 -
9.676  -3.915  1.00  0.00      BrD ATOM    373  O   LEU   22       0.086 -
9.813  -4.295  1.00  0.00      BrD ATOM    374  N   GLN   23       2.201 -
10.552  -4.058  1.00  0.00     BrD ATOM    375  HN  GLN   23       3.107 -
10.354  -3.735  1.00  0.00     BrD ATOM    376  CA  GLN   23       1.941 -
11.841  -4.693  1.00  0.00     BrD ATOM    377  HA  GLN   23       1.828 -
11.670  -5.754  1.00  0.00     BrD ATOM    378  CB  GLN   23       3.118 -
12.793  -4.464  1.00  0.00     BrD ATOM    379  HB1 GLN   23       3.720 -
12.412  -3.653  1.00  0.00     BrD ATOM    380  HB2 GLN   23       2.731 -
13.763  -4.186  1.00  0.00     BrD ATOM    381  CG  GLN   23       4.012 -
12.969  -5.682  1.00  0.00     BrD ATOM    382  HG1 GLN   23       4.318 -
11.995  -6.035  1.00  0.00     BrD ATOM    383  HG2 GLN   23       4.886 -
13.535  -5.393  1.00  0.00     BrD ATOM    384  CD  GLN   23       3.316 -
13.697  -6.815  1.00  0.00     BrD ATOM    385  OE1 GLN   23       2.624 -
14.692  -6.597  1.00  0.00     BrD ATOM    386  NE2 GLN   23       3.494 -
13.203  -8.034  1.00  0.00     BrD ATOM    387  HE21 GLN  23       4.058 -
12.408  -8.134  1.00  0.00     BrD ATOM    388  HE22 GLN  23       3.055 -
13.654  -8.786  1.00  0.00     BrD ATOM    389  C   GLN   23       0.655 -
12.467  -4.157  1.00  0.00     BrD ATOM    390  O   GLN   23      -0.207 -
12.892  -4.925  1.00  0.00     BrD ATOM    391  N   GLN   24       0.530 -
12.519  -2.833  1.00  0.00     BrD ATOM    392  HN  GLN   24       1.252 -
12.167  -2.269  1.00  0.00     BrD ATOM    393  CA  GLN   24      -0.654 -
13.096  -2.203  1.00  0.00     BrD ATOM    394  HA  GLN   24      -0.951 -
13.947  -2.797  1.00  0.00     BrD ATOM    395  CB  GLN   24      -0.325 -
13.584  -0.783  1.00  0.00     BrD ATOM    396  HB1 GLN   24       0.666 -
14.012  -0.785  1.00  0.00     BrD ATOM    397  HB2 GLN   24      -1.035 -
14.351  -0.509  1.00  0.00     BrD ATOM    398  CG  GLN   24      -0.369 -
12.498   0.284  1.00  0.00     BrD ATOM    399  HG1 GLN   24      -1.331 -
12.531   0.774  1.00  0.00     BrD ATOM    400  HG2 GLN   24      -0.243 -
11.539  -0.192  1.00  0.00     BrD ATOM    401  CD  GLN   24       0.714 -
13.663   1.333  1.00  0.00     BrD ATOM    402  OE1 GLN   24       0.426 -
12.791   2.524  1.00  0.00     BrD ATOM    403  NE2 GLN   24       1.967 -
12.659   0.697  1.00  0.00     BrD ATOM    404  HE21 GLN  24       2.122 -
12.552  -0.065  1.00  0.00     BrD ATOM    405  HE22 GLN  24       2.687 -
12.763   1.554  1.00  0.00     BrD ATOM    406  C   GLN   24      -1.816 -
12.099  -2.179  1.00  0.00     BrD ATOM    407  O   GLN   24      -2.974 -
12.485  -2.331  1.00  0.00     BrD ATOM    408  N   VAL   25      -1.501 -
10.821  -1.974  1.00  0.00     BrD ATOM    409  HN  VAL   25      -0.561 -
10.575  -1.859  1.00  0.00     BrD ATOM    410  CA  VAL   25      -2.523 -
9.776  -1.922  1.00  0.00      BrD ATOM    411  HA  VAL   25      -3.121 -
9.941  -1.036  1.00  0.00      BrD ATOM    412  CB  VAL   25      -1.890 -
8.369  -1.813  1.00  0.00      BrD ATOM    413  HB  VAL   25      -1.198 -
8.243  -2.632  1.00  0.00      BrD ATOM    414  CG1 VAL   25      -1.116 -
8.236  -0.510  1.00  0.00      BrD ATOM    415  HG11 VAL  25      -1.590 -
7.494   0.116  1.00  0.00      BrD ATOM    416  HG12 VAL  25      -0.102 -
7.932  -0.722  1.00  0.00      BrD ATOM    417  HG13 VAL  25      -1.108 -
9.186   0.003  1.00  0.00      BrD ATOM    418  CG2 VAL   25      -2.965 -
7.277  -1.908  1.00  0.00      BrD ATOM    419  HG21 VAL  25      -3.437 -
7.331  -2.668  1.00  0.00      BrD ATOM    420  HG22 VAL  25      -2.472 -
6.313  -1.799  1.00  0.00      BrD ATOM    421  HG23 VAL  25      -3.672 -
7.410  -1.121  1.00  0.00      BrD ATOM    422  C   VAL   25      -3.440 -
9.846  -3.161  1.00  0.00      BrD ATOM    423  O   VAL   25      -4.659 -
9.930  -3.000  1.00  0.00      BrD ATOM    424  N   LYS   26      -2.858 -
9.858  -4.336  1.00  0.00      BrD ATOM    425  HN  LYS   26      -1.883 -
9.798  -4.396  1.00  0.00      BrD ATOM    426  CA  LYS   26      -3.648 -
9.943  -5.562  1.00  0.00      BrD ATOM    427  HA  LYS   26      -4.174 -
9.008  -5.676  1.00  0.00      BrD ATOM    428  CB  LYS   26      -2.737 -
10.161  -6.771  1.00  0.00     BrD ATOM    429  HB1 LYS   26      -3.314 -
10.018  -7.673  1.00  0.00     BrD ATOM    430  HB2 LYS   26      -1.942 -
9.430  -6.744  1.00  0.00      BrD ATOM    431  CG  LYS   26      -2.111 -
11.548  -6.820  1.00  0.00     BrD ATOM    432  HG1 LYS   26      -2.070 -
11.947  -5.818  1.00  0.00     BrD ATOM    433  HG2 LYS   26      -2.721 -
12.183  -7.442  1.00  0.00     BrD ATOM    434  CD  LYS   26      -0.702 -
11.500  -7.391  1.00  0.00     BrD ATOM    435  HD1 LYS   26      -0.214 -
10.600  -7.048  1.00  0.00     BrD ATOM    436  HD2 LYS   26      -0.156 -
12.364  -7.043  1.00  0.00     BrD ATOM    437  CE  LYS   26      -0.716 -
11.505  -8.910  1.00  0.00     BrD ATOM    438  HE1 LYS   26       0.003 -
10.782  -9.266  1.00  0.00     BrD ATOM    439  HE2 LYS   26      -1.703 -
11.228  -9.249  1.00  0.00     BrD ATOM    440  NZ  LYS   26      -0.371 -
12.844  -3.465  1.00  0.00     BrD ATOM    441  HZ1 LYS   26      -1.216 -
13.285  -3.884  1.00  0.00     BrD ATOM    442  HZ2 LYS   26      -0.010 -
13.461  -4.710  1.00  0.00     BrD ATOM    443  HZ3 LYS   26       0.356 -
12.749 -10.199  1.00  0.00     BrD ATOM    444  C   LYS   26      -4.673 -
11.073  -5.468  1.00  0.00     BrD ATOM    445  O   LYS   26      -5.762 -
10.991  -6.036  1.00  0.00     BrD ATOM    446  N   SER   27      -4.315 -
12.118  -4.732  1.00  0.00     BrD ATOM    447  HN  SER   27      -3.439 -
12.109  -4.293  1.00  0.00     BrD ATOM    448  CA  SER   27      -5.204 -
13.257  -4.516  1.00  0.00     BrD ATOM    449  HA  SER   27      -6.104 -
13.100  -5.091  1.00  0.00     BrD ATOM    450  CB  SER   27      -4.532 -
14.553  -4.976  1.00  0.00     BrD ATOM    451  HB1 SER   27      -3.639 -
14.710  -4.404  1.00  0.00     BrD ATOM    452  HB2 SER   27      -5.207 -
15.381  -4.818  1.00  0.00     BrD ATOM    453  OG  SER   27      -4.197 -
14.492  -6.351  1.00  0.00     BrD ATOM    454  HG  SER   27      -3.746 -
15.300  -6.606  1.00  0.00     BrD ATOM    455  C   SER   27      -5.591 -
13.361  -3.050  1.00  0.00     BrD ATOM    456  O   SER   27      -5.962 -
14.431  -2.567  1.00  0.00     BrD ATOM    457  N   HIS   28      -5.477 -
12.246  -2.339  1.00  0.00     BrD ATOM    458  HN  HIS   28      -5.215 -
11.418  -2.785  1.00  0.00     BrD ATOM    459  CA  HIS   28      -5.863 -
12.197  -0.946  1.00  0.00     BrD ATOM    460  HA  HIS   28      -5.597 -
13.142  -0.497  1.00  0.00     BrD ATOM    461  CB  HIS   28      -5.125 -
11.076  -0.217  1.00  0.00     BrD ATOM    462  HB1 HIS   28      -4.073 -
11.308  -0.210  1.00  0.00     BrD ATOM    463  HB2 HIS   28      -5.283 -
10.146  -0.742  1.00  0.00     BrD ATOM    464  CG  HIS   28      -5.549 -
10.884   1.205  1.00  0.00     BrD ATOM    465  ND1 HIS   28      -5.742 -
11.931   2.081  1.00  0.00     BrD ATOM    466  HD1 HIS   28      -5.648 -
12.883   1.866  1.00  0.00     BrD ATOM    467  CD2 HIS   28      -5.780 -
9.754   1.916  1.00  0.00      BrD ATOM    468  HD2 HIS   28      -5.717 -
8.739   1.549  1.00  0.00      BrD ATOM    469  CE1 HIS   28      -6.092 -
11.456   3.262  1.00  0.00     BrD ATOM    470  HE1 HIS   28      -6.314 -
12.044   4.141  1.00  0.00     BrD ATOM    471  NE2 HIS   28      -6.119 -
10.139   3.189  1.00  0.00     BrD ATOM    472  HE2 HIS   28      -6.350 -
9.536   3.925  1.00  0.00      BrD ATOM    473  C   HIS   28      -7.364 -
12.017  -0.850  1.00  0.00     BrD ATOM    474  O   HIS   28      -7.979 -
11.356  -1.686  1.00  0.00     BrD ATOM    475  N   GLN   29      -7.954 -
12.666   0.128  1.00  0.00     BrD ATOM    476  HN  GLN   29      -7.404 -
13.189   0.747  1.00  0.00     BrD ATOM    477  CA  GLN   29      -9.397 -
12.630   0.298  1.00  0.00     BrD ATOM    478  HA  GLN   29      -9.836 -
12.688  -0.687  1.00  0.00     BrD ATOM    479  CB  GLN   29      -9.840 -
13.850   1.090  1.00  0.00     BrD ATOM    480  HB1 GLN   29      -9.485 -
13.761   2.106  1.00  0.00     BrD ATOM    481  HB2 GLN   29     -10.918 -
13.901   1.092  1.00  0.00     BrD ATOM    482  CG  GLN   29      -9.294 -
15.138   0.496  1.00  0.00     BrD ATOM    483  HG1 GLN   29      -8.707 -
14.887  -0.386  1.00  0.00     BrD ATOM    484  HG2 GLN   29      -8.660 -
15.618   1.227  1.00  0.00     BrD ATOM    485  CD  GLN   29     -10.390 -
16.105   0.093  1.00  0.00     BrD ATOM    486  OE1 GLN   29     -10.358 -
16.479  -0.996  1.00  0.00     BrD ATOM    487  NE2 GLN   29     -11.368 -
16.290   0.971  1.00  0.00     BrD ATOM    488  HE21 GLN  29     -12.090 -
16.910   0.737  1.00  0.00     BrD ATOM    489  HE22 GLN  29     -11.329 -
15.800   1.819  1.00  0.00     BrD ATOM    490  C   GLN   29      -9.866 -
11.332   0.951  1.00  0.00     BrD ATOM    491  O   GLN   29     -11.065 -
11.111   1.116  1.00  0.00     BrD ATOM    492  N   SER   30      -8.921 -
10.450   1.262  1.00  0.00     BrD ATOM    493  HN  SER   30      -7.985 -
10.661   1.074  1.00  0.00     BrD ATOM    494  CA  SER   30      -9.246 -
9.143   1.805  1.00  0.00      BrD ATOM    495  HA  SER   30     -10.319 -
9.036   1.787  1.00  0.00      BrD ATOM    496  CB  SER   30      -8.759 -
9.026   3.250  1.00  0.00      BrD ATOM    497  HB1 SER   30      -7.829 -
8.479   3.271  1.00  0.00      BrD ATOM    498  HB2 SER   30      -9.499 -
8.500   3.835  1.00  0.00      BrD ATOM    499  OG  SER   30      -8.552 -
10.307   3.823  1.00  0.00     BrD ATOM    500  HG  SER   30      -9.332 -
10.857   3.664  1.00  0.00     BrD ATOM    501  C   SER   30      -8.637 -
8.036   0.965  1.00  0.00      BrD ATOM    502  O   SER   30      -8.726 -
6.855   1.276  1.00  0.00      BrD ATOM    503  N   ALA   31      -7.977 -
8.425  -0.157  1.00  0.00      BrD ATOM    504  HN  ALA   31      -7.935 -
9.377  -0.385  1.00  0.00      BrD ATOM    505  CA  ALA   31      -7.365 -
7.462  -1.066  1.00  0.00      BrD ATOM    506  HA  ALA   31      -6.927 -
6.675  -0.470  1.00  0.00      BrD ATOM    507  CB  ALA   31      -6.251 -
8.123  -1.861  1.00  0.00      BrD ATOM    508  HB1 ALA   31      -5.395 -
8.274  -1.223  1.00  0.00      BrD ATOM    509  HB2 ALA   31      -5.974 -
7.489  -2.691  1.00  0.00      BrD ATOM    510  HB3 ALA   31      -6.593 -
9.076  -2.236  1.00  0.00      BrD ATOM    511  C   ALA   31      -8.397 -
6.851  -2.014  1.00  0.00      BrD ATOM    512  O   ALA   31      -8.097 -
5.900  -2.726  1.00  0.00      BrD ATOM    513  N   TRP   32      -9.614 -
7.396  -2.010  1.00  0.00      BrD ATOM    514  HN  TRP   32      -9.795 -
8.160  -1.427  1.00  0.00      BrD ATOM    515  CA  TRP   32     -10.669 -
6.906  -2.893  1.00  0.00      BrD ATOM    516  HA  TRP   32     -10.362 -
7.135  -3.902  1.00  0.00      BrD ATOM    517  CB  TRP   32     -12.002 -
7.630  -2.628  1.00  0.00      BrD ATOM    518  HB1 TRP   32     -12.770 -
7.192  -3.249  1.00  0.00      BrD ATOM    519  HB2 TRP   32     -11.894 -
6.671  -2.881  1.00  0.00      BrD ATOM    520  CG  TRP   32     -12.454 -
7.544  -1.209  1.00  0.00      BrD ATOM    521  CD1 TRP   32     -12.415 -
8.532  -0.267  1.00  0.00      BrD ATOM    522  HD1 TRP   32     -12.058 -
9.535  -0.450  1.00  0.00      BrD ATOM    523  CD2 TRP   32     -12.993 -
6.391  -0.565  1.00  0.00      BrD ATOM    524  NE1 TRP   32     -12.895 -
8.057   0.929  1.00  0.00      BrD ATOM    525  HE1 TRP   32     -12.970 -
8.574   1.758  1.00  0.00      BrD ATOM    526  CE2 TRP   32     -13.253 -
6.743   0.770  1.00  0.00      BrD ATOM    527  CE3 TRP   32     -13.270 -
5.095  -0.991  1.00  0.00      BrD ATOM    528  HE3 TRP   32     -13.068 -
4.788  -2.006  1.00  0.00      BrD ATOM    529  CZ2 TRP   32     -13.784 -
5.839   1.681  1.00  0.00      BrD ATOM    530  HZ2 TRP   32     -13.983 -
6.109   2.708  1.00  0.00      BrD ATOM    531  CZ3 TRP   32     -13.786 -
4.198  -0.084  1.00  0.00      BrD ATOM    532  HZ3 TRP   32     -14.003 -
3.185  -0.396  1.00  0.00      BrD ATOM    533  CH2 TRP   32     -14.055 -
4.577   1.230  1.00  0.00      BrD ATOM    534  HH2 TRP   32     -14.420 -
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3.838   1.903  1.00  0.00      BrD ATOM    535  C    TRP   32     -10.855  -
5.382  -2.797  1.00  0.00      BrD ATOM    536  O    TRP   32     -11.199  -
4.752  -3.797  1.00  0.00      BrD ATOM    537  N    PRO   33     -10.636  -
4.741  -1.618  1.00  0.00      BrD ATOM    538  CA   PRO   33     -10.800  -
3.297  -1.493  1.00  0.00      BrD ATOM    539  HA   PRO   33     -11.693  -
2.959  -1.999  1.00  0.00      BrD ATOM    540  CB   PRO   33     -10.947  -
3.057   0.017  1.00  0.00      BrD ATOM    541  HB1  PRO   33     -10.191  -
2.357   0.341  1.00  0.00      BrD ATOM    542  HB2  PRO   33     -11.926  -
2.646   0.219  1.00  0.00      BrD ATOM    543  CG   PRO   33     -10.771  -
4.386   0.685  1.00  0.00      BrD ATOM    544  HG1  PRO   33     -11.713  -
4.744   1.048  1.00  0.00      BrD ATOM    545  HG2  PRO   33     -10.075  -
4.288   1.505  1.00  0.00      BrD ATOM    546  CD   PRO   33     -10.223  -
5.331  -0.337  1.00  0.00      BrD ATOM    547  HD1  PRO   33     -10.632  -
6.319  -0.205  1.00  0.00      BrD ATOM    548  HD2  PRO   33      -9.165  -
5.358  -0.254  1.00  0.00      BrD ATOM    549  C    PRO   33      -9.596  -
2.535  -2.040  1.00  0.00      BrD ATOM    550  O    PRO   33      -9.687  -
1.343  -2.332  1.00  0.00      BrD ATOM    551  N    PHE   34      -8.472  -
3.233  -2.187  1.00  0.00      BrD ATOM    552  HN   PHE   34      -8.458  -
4.180  -1.936  1.00  0.00      BrD ATOM    553  CA   PHE   34      -7.256  -
2.619  -2.703  1.00  0.00      BrD ATOM    554  HA   PHE   34      -7.295  -
1.564  -2.475  1.00  0.00      BrD ATOM    555  CB   PHE   34      -6.026  -
3.228  -3.030  1.00  0.00      BrD ATOM    556  HB1  PHE   34      -5.773  -
4.150  -2.531  1.00  0.00      BrD ATOM    557  HB2  PHE   34      -5.198  -
2.540  -3.118  1.00  0.00      BrD ATOM    558  CG   PHE   34      -6.226  -
3.531  -0.573  1.00  0.00      BrD ATOM    559  CD1  PHE   34      -6.985  -
2.689   0.226  1.00  0.00      BrD ATOM    560  HD1  PHE   34      -7.430  -
1.805  -0.208  1.00  0.00      BrD ATOM    561  CD2  PHE   34      -5.663  -
4.659  -0.003  1.00  0.00      BrD ATOM    562  HD2  PHE   34      -5.074  -
5.324  -0.617  1.00  0.00      BrD ATOM    563  CE1  PHE   34      -7.175  -
2.968   1.566  1.00  0.00      BrD ATOM    564  HE1  PHE   34      -7.767  -
2.303   2.179  1.00  0.00      BrD ATOM    565  CE2  PHE   34      -5.852  -
4.944   1.335  1.00  0.00      BrD ATOM    566  HE2  PHE   34      -5.409  -
5.829   1.765  1.00  0.00      BrD ATOM    567  CZ   PHE   34      -6.607  -
4.098   2.122  1.00  0.00      BrD ATOM    568  HZ   PHE   34      -6.753  -
4.319   3.168  1.00  0.00      BrD ATOM    569  C    PHE   34      -7.150  -
2.790  -4.213  1.00  0.00      BrD ATOM    570  O    PHE   34      -6.653  -
1.909  -4.907  1.00  0.00      BrD ATOM    571  N    MET   35      -7.624  -
3.921  -4.721  1.00  0.00      BrD ATOM    572  HN   MET   35      -8.000  -
4.598  -4.119  1.00  0.00      BrD ATOM    573  CA   MET   35      -7.545  -
4.205  -6.151  1.00  0.00      BrD ATOM    574  HA   MET   35      -6.600  -
3.825  -6.507  1.00  0.00      BrD ATOM    575  CB   MET   35      -7.593  -
5.706  -6.393  1.00  0.00      BrD ATOM    576  HB1  MET   35      -7.670  -
5.889  -7.454  1.00  0.00      BrD ATOM    577  HB2  MET   35      -8.463  -
6.114  -5.699  1.00  0.00      BrD ATOM    578  CG   MET   35      -6.367  -
6.423  -5.471  1.00  0.00      BrD ATOM    579  HG1  MET   35      -6.673  -
7.114  -5.107  1.00  0.00      BrD ATOM    580  HG2  MET   35      -5.696  -
5.692  -5.444  1.00  0.00      BrD ATOM    581  SD   MET   35      -5.490  -
7.322  -7.161  1.00  0.00      BrD ATOM    582  CE   MET   35      -4.032  -
6.298  -7.337  1.00  0.00      BrD ATOM    583  HE1  MET   35      -3.284  -
6.831  -7.905  1.00  0.00      BrD ATOM    584  HE2  MET   35      -3.639  -
6.062  -6.358  1.00  0.00      BrD ATOM    585  HE3  MET   35      -4.294  -
5.384  -7.850  1.00  0.00      BrD ATOM    586  C    MET   35      -8.661  -
3.519  -6.924  1.00  0.00      BrD ATOM    587  O    MET   35      -9.396  -
4.160  -7.675  1.00  0.00      BrD ATOM    588  N    GLU   36      -8.749  -
2.208  -6.762  1.00  0.00      BrD ATOM    589  HN   GLU   36      -8.116  -
1.765  -6.164  1.00  0.00      BrD ATOM    590  CA   GLU   36      -9.751  -
1.407  -7.457  1.00  0.00      BrD ATOM    591  HA   GLU   36      -9.531  -
1.453  -8.515  1.00  0.00      BrD ATOM    592  CB   GLU   36     -11.156  -
1.964  -7.207  1.00  0.00      BrD ATOM    593  HB1  GLU   36     -11.084  -
2.018  -6.987  1.00  0.00      BrD ATOM    594  HB2  GLU   36     -11.581  -
1.458  -6.354  1.00  0.00      BrD ATOM    595  CG   GLU   36     -12.099  -
1.787  -8.385  1.00  0.00      BrD ATOM    596  HG1  GLU   36     -11.527  -
1.466  -9.243  1.00  0.00      BrD ATOM    597  HG2  GLU   36     -12.569  -
2.735  -8.600  1.00  0.00      BrD ATOM    598  CD   GLU   36     -13.182  -
0.761  -8.114  1.00  0.00      BrD ATOM    599  OE1  GLU   36     -12.865
0.447  -8.098  1.00  0.00      BrD ATOM    600  OE2  GLU   36     -14.348  -
1.165  -7.919  1.00  0.00      BrD ATOM    601  C    GLU   36      -9.692
0.050  -7.001  1.00  0.00      BrD ATOM    602  O    GLU   36     -10.470
0.471  -6.145  1.00  0.00      BrD ATOM    603  N    PRO   37      -8.764
0.842  -7.565  1.00  0.00      BrD ATOM    604  CA   PRO   37      -8.604
2.255  -7.202  1.00  0.00      BrD ATOM    605  HA   PRO   37      -8.407
2.369  -6.146  1.00  0.00      BrD ATOM    606  CB   PRO   37      -7.376
2.709  -8.004  1.00  0.00      BrD ATOM    607  HB1  PRO   37      -7.696
3.306  -8.846  1.00  0.00      BrD ATOM    608  HB2  PRO   37      -6.728
3.295  -7.370  1.00  0.00      BrD ATOM    609  CG   PRO   37      -6.706
1.453  -8.451  1.00  0.00      BrD ATOM    610  HG1  PRO   37      -6.222
1.614  -9.403  1.00  0.00      BrD ATOM    611  HG2  PRO   37      -5.984
1.139  -7.711  1.00  0.00      BrD ATOM    612  CD   PRO   37      -7.793
0.426  -8.587  1.00  0.00      BrD ATOM    613  HD1  PRO   37      -8.229
0.465  -9.574  1.00  0.00      BrD ATOM    614  HD2  PRO   37      -7.410  -
0.561  -8.378  1.00  0.00      BrD ATOM    615  C    PRO   37      -9.822
3.093  -7.576  1.00  0.00      BrD ATOM    616  O    PRO   37     -10.678
2.655  -8.344  1.00  0.00      BrD ATOM    617  N    VAL   38      -9.892
4.301  -7.025  1.00  0.00      BrD ATOM    618  HN   VAL   38      -9.179
4.594  -6.422  1.00  0.00      BrD ATOM    619  CA   VAL   38     -11.006
5.206  -7.300  1.00  0.00      BrD ATOM    620  HA   VAL   38     -11.709
4.683  -7.931  1.00  0.00      BrD ATOM    621  CB   VAL   38     -11.750
5.646  -6.012  1.00  0.00      BrD ATOM    622  HB   VAL   38     -11.449
6.657  -5.781  1.00  0.00      BrD ATOM    623  CG1  VAL   38     -11.395
4.767  -4.819  1.00  0.00      BrD ATOM    624  HG11 VAL   38     -11.888
5.145  -3.935  1.00  0.00      BrD ATOM    625  HG12 VAL   38     -10.326
4.779  -4.667  1.00  0.00      BrD ATOM    626  HG13 VAL   38     -11.721
3.755  -5.008  1.00  0.00      BrD ATOM    627  CG2  VAL   38     -13.253
5.646  -6.246  1.00  0.00      BrD ATOM    628  HG21 VAL   38     -13.760

5.374  -5.333  1.00  0.00      BrD ATOM    629  HG22 VAL   38     -13.497
4.934  -7.020  1.00  0.00      BrD ATOM    630  HG23 VAL   38     -13.570
6.629  -6.553  1.00  0.00      BrD ATOM    631  C    VAL   38     -10.516
6.451  -8.035  1.00  0.00      BrD ATOM    632  O    VAL   38      -9.410
6.473  -8.571  1.00  0.00      BrD ATOM    633  N    LYS   39     -11.349
7.488  -8.051  1.00  0.00      BrD ATOM    634  HN   LYS   39     -12.215
7.412  -7.609  1.00  0.00      BrD ATOM    635  CA   LYS   39     -11.005
8.737  -8.715  1.00  0.00      BrD ATOM    636  HA   LYS   39      -9.947
8.906  -8.574  1.00  0.00      BrD ATOM    637  CB   LYS   39     -11.299
8.646 -10.216  1.00  0.00      BrD ATOM    638  HB1  LYS   39     -10.419
8.285 -10.714  1.00  0.00      BrD ATOM    639  HB2  LYS   39     -11.531
9.633 -10.587  1.00  0.00      BrD ATOM    640  CG   LYS   39     -12.452
7.722 -10.569  1.00  0.00      BrD ATOM    641  HG1  LYS   39     -12.970
7.450  -9.664  1.00  0.00      BrD ATOM    642  HG2  LYS   39     -13.127
8.241 -11.232  1.00  0.00      BrD ATOM    643  CD   LYS   39     -11.962
6.458 -11.256  1.00  0.00      BrD ATOM    644  HD1  LYS   39     -12.413
5.601 -10.777  1.00  0.00      BrD ATOM    645  HD2  LYS   39     -10.888
6.402 -11.160  1.00  0.00      BrD ATOM    646  CE   LYS   39     -12.326
6.447 -12.732  1.00  0.00      BrD ATOM    647  HE1  LYS   39     -11.779
5.653 -13.219  1.00  0.00      BrD ATOM    648  HE2  LYS   39     -12.044
7.395 -13.166  1.00  0.00      BrD ATOM    649  NZ   LYS   39     -13.784
6.232 -12.945  1.00  0.00      BrD ATOM    650  HZ1  LYS   39     -13.963
5.950 -13.930  1.00  0.00      BrD ATOM    651  HZ2  LYS   39     -14.307
7.108 -12.745  1.00  0.00      BrD ATOM    652  HZ3  LYS   39     -14.130
5.482 -12.313  1.00  0.00      BrD ATOM    653  C    LYS   39     -11.772
9.903  -8.105  1.00  0.00      BrD ATOM    654  O    LYS   39     -12.487
9.739  -7.116  1.00  0.00      BrD ATOM    655  N    ARG   40     -11.626
11.078  -8.706  1.00  0.00      BrD ATOM    656  HN   ARG   40     -11.040
11.146  -9.488  1.00  0.00      BrD ATOM    657  CA   ARG   40     -12.306
12.273  -8.223  1.00  0.00      BrD ATOM    658  HA   ARG   40     -12.018
12.419  -7.191  1.00  0.00      BrD ATOM    659  CB   ARG   40     -11.866
13.492  -9.017  1.00  0.00      BrD ATOM    660  HB1  ARG   40     -12.313
13.435 -10.019  1.00  0.00      BrD ATOM    661  HB2  ARG   40     -10.792
13.476  -9.139  1.00  0.00      BrD ATOM    662  CG   ARG   40     -12.265
14.819  -8.410  1.00  0.00      BrD ATOM    663  HG1  ARG   40     -12.664
14.634  -7.424  1.00  0.00      BrD ATOM    664  HG2  ARG   40     -13.020
15.265  -9.025  1.00  0.00      BrD ATOM    665  CD   ARG   40     -11.075
15.759  -8.292  1.00  0.00      BrD ATOM    666  HD1  ARG   40     -10.715
15.948  -9.284  1.00  0.00      BrD ATOM    667  HD2  ARG   40     -10.296
15.263  -7.732  1.00  0.00      BrD ATOM    668  NE   ARG   40     -11.426
17.004  -7.616  1.00  0.00      BrD ATOM    669  HE   ARG   40     -11.554
17.802  -8.171  1.00  0.00      BrD ATOM    670  CZ   ARG   40     -11.577
17.109  -6.300  1.00  0.00      BrD ATOM    671  NH1  ARG   40     -11.409
16.047  -5.525  1.00  0.00      BrD ATOM    672  NH11 ARG   40     -11.168
15.165  -5.930  1.00  0.00      BrD ATOM    673  NH12 ARG   40     -11.523
16.127  -4.535  1.00  0.00      BrD ATOM    674  NH2  ARG   40     -11.897
18.276  -5.758  1.00  0.00      BrD ATOM    675  NH21 ARG   40     -12.011
18.353  -4.767  1.00  0.00      BrD ATOM    676  NH22 ARG   40     -12.025
19.079  -6.139  1.00  0.00      BrD ATOM    677  C    ARG   40     -13.824
12.123  -8.293  1.00  0.00      BrD ATOM    678  O    ARG   40     -14.556
12.915  -7.700  1.00  0.00      BrD ATOM    679  N    THR   41     -14.301
11.109  -9.017  1.00  0.00      BrD ATOM    680  HN   THR   41     -13.680
10.511  -9.481  1.00  0.00      BrD ATOM    681  CA   THR   41     -15.727
10.898  -9.159  1.00  0.00      BrD ATOM    682  HA   THR   41     -16.228
11.725  -8.681  1.00  0.00      BrD ATOM    683  CB   THR   41     -16.133
10.870 -10.637  1.00  0.00      BrD ATOM    684  HB   THR   41     -15.862
11.812 -11.090  1.00  0.00      BrD ATOM    685  OG1  THR   41     -17.533
10.696 -10.775  1.00  0.00      BrD ATOM    686  HG1  THR   41     -17.988
11.239 -10.127  1.00  0.00      BrD ATOM    687  CG2  THR   41     -15.453
9.771 -11.421  1.00  0.00      BrD ATOM    688  HG21 THR   41     -14.433
9.669 -11.083  1.00  0.00      BrD ATOM    689  HG22 THR   41     -15.462
10.020 -12.472  1.00  0.00      BrD ATOM    690  HG23 THR   41     -15.979
8.841 -11.267  1.00  0.00      BrD ATOM    691  C    THR   41     -16.197
9.623  -8.467  1.00  0.00      BrD ATOM    692  O    THR   41     -17.123
9.656  -7.658  1.00  0.00      BrD ATOM    693  N    GLU   42     -15.573
8.498  -8.792  1.00  0.00      BrD ATOM    694  HN   GLU   42     -14.835
8.521  -9.435  1.00  0.00      BrD ATOM    695  CA   GLU   42     -15.940
7.236  -8.163  1.00  0.00      BrD ATOM    696  HA   GLU   42     -16.954
7.002  -8.454  1.00  0.00      BrD ATOM    697  CB   GLU   42     -15.013
6.109  -8.623  1.00  0.00      BrD ATOM    698  HB1  GLU   42     -15.239
5.220  -8.053  1.00  0.00      BrD ATOM    699  HB2  GLU   42     -13.993
6.398  -8.431  1.00  0.00      BrD ATOM    700  CG   GLU   42     -15.142
5.774 -10.098  1.00  0.00      BrD ATOM    701  HG1  GLU   42     -14.284
5.191 -10.396  1.00  0.00      BrD ATOM    702  HG2  GLU   42     -15.166
6.694 -10.663  1.00  0.00      BrD ATOM    703  CD   GLU   42     -16.397
4.982 -10.409  1.00  0.00      BrD ATOM    704  OE1  GLU   42     -17.489
5.589 -10.443  1.00  0.00      BrD ATOM    705  OE2  GLU   42     -16.289
3.756 -10.620  1.00  0.00      BrD ATOM    706  C    GLU   42     -15.881
7.374  -6.647  1.00  0.00      BrD ATOM    707  O    GLU   42     -16.614
6.703  -5.920  1.00  0.00      BrD ATOM    708  N    ALA   43     -15.024
8.279  -6.181  1.00  0.00      BrD ATOM    709  HN   ALA   43     -14.457
8.774  -6.817  1.00  0.00      BrD ATOM    710  CA   ALA   43     -14.861
8.509  -4.752  1.00  0.00      BrD ATOM    711  HA   ALA   43     -15.712
8.080  -4.245  1.00  0.00      BrD ATOM    712  CB   ALA   43     -13.609
7.810  -4.245  1.00  0.00      BrD ATOM    713  HB1  ALA   43     -12.893
7.721  -5.049  1.00  0.00      BrD ATOM    714  HB2  ALA   43     -13.866
6.823  -3.893  1.00  0.00      BrD ATOM    715  HB3  ALA   43     -13.180
8.381  -3.435  1.00  0.00      BrD ATOM    716  C    ALA   43     -14.799
10.002  -4.440  1.00  0.00      BrD ATOM    717  O    ALA   43     -13.721
10.555  -4.222  1.00  0.00      BrD ATOM    718  N    PRO   44     -15.962
10.676  -4.414  1.00  0.00      BrD ATOM    719  CA   PRO   44     -16.038
12.114  -4.129  1.00  0.00      BrD ATOM    720  HA   PRO   44     -15.511
12.692  -4.874  1.00  0.00      BrD ATOM    721  CB   PRO   44     -17.939
12.422  -4.207  1.00  0.00      BrD ATOM    722  HB1  PRO   44     -17.688

11.369  -4.704  1.00  0.00      BrD ATOM    723  HB2  PRO   44     -17.951
12.465  -3.210  1.00  0.00      BrD ATOM    724  CG   PRO   44     -18.125
11.298  -4.991  1.00  0.00      BrD ATOM    725  HG1  PRO   44     -18.071
11.518  -6.047  1.00  0.00      BrD ATOM    726  HG2  PRO   44     -19.150
11.137  -4.692  1.00  0.00      BrD ATOM    727  CD   PRO   44     -17.291
10.095  -4.665  1.00  0.00      BrD ATOM    728  HD1  PRO   44     -17.264
9.413  -5.500  1.00  0.00      BrD ATOM    729  HD2  PRO   44     -17.668
9.601  -3.783  1.00  0.00      BrD ATOM    730  C    PRO   44     -15.498
12.458  -2.746  1.00  0.00      BrD ATOM    731  O    PRO   44     -16.262
12.635  -1.797  1.00  0.00      BrD ATOM    732  N    GLY   45     -14.177
12.551  -2.637  1.00  0.00      BrD ATOM    733  HN   GLY   45     -13.617
12.400  -3.427  1.00  0.00      BrD ATOM    734  CA   GLY   45     -13.560
12.675  -1.365  1.00  0.00      BrD ATOM    735  HA1  GLY   45     -13.586
13.946  -1.228  1.00  0.00      BrD ATOM    736  HA2  GLY   45     -14.128
12.409  -0.573  1.00  0.00      BrD ATOM    737  C    GLY   45     -12.121
12.405  -1.278  1.00  0.00      BrD ATOM    738  O    GLY   45     -11.333
12.942  -0.499  1.00  0.00      BrD ATOM    739  N    TYR   46     -11.777
11.403  -2.081  1.00  0.00      BrD ATOM    740  HN   TYR   46     -12.450
11.015  -2.678  1.00  0.00      BrD ATOM    741  CA   TYR   46     -10.423
10.861  -2.089  1.00  0.00      BrD ATOM    742  HA   TYR   46     -10.271
10.337  -1.158  1.00  0.00      BrD ATOM    743  CB   TYR   46     -10.255
9.478  -3.249  1.00  0.00      BrD ATOM    744  HB1  TYR   46     -11.073
10.006  -3.942  1.00  0.00      BrD ATOM    745  HB2  TYR   46      -9.324
10.084  -3.755  1.00  0.00      BrD ATOM    746  CG   TYR   46     -10.237
8.431  -2.814  1.00  0.00      BrD ATOM    747  CD1  TYR   46      -9.362
7.558  -3.279  1.00  0.00      BrD ATOM    748  HD1  TYR   46      -8.511
7.926  -3.962  1.00  0.00      BrD ATOM    749  CD2  TYR   46     -11.194
7.938  -1.935  1.00  0.00      BrD ATOM    750  HD2  TYR   46     -11.958
8.605  -1.564  1.00  0.00      BrD ATOM    751  CE1  TYR   46      -9.242
6.235  -2.884  1.00  0.00      BrD ATOM    752  HE1  TYR   46      -8.474
5.572  -3.254  1.00  0.00      BrD ATOM    753  CE2  TYR   46     -11.180
6.617  -1.534  1.00  0.00      BrD ATOM    754  HE2  TYR   46     -11.933
6.253  -0.850  1.00  0.00      BrD ATOM    755  CZ   TYR   46     -10.203
5.769  -2.010  1.00  0.00      BrD ATOM    756  OH   TYR   46     -10.186
4.452  -1.612  1.00  0.00      BrD ATOM    757  HH   TYR   46      -9.895
4.397  -0.699  1.00  0.00      BrD ATOM    758  C    TYR   46      -9.386
11.975  -2.200  1.00  0.00      BrD ATOM    759  O    TYR   46      -9.727
13.132  -2.446  1.00  0.00      BrD ATOM    760  N    TYR   47      -8.120
11.618  -2.014  1.00  0.00      BrD ATOM    761  HN   TYR   47      -7.911
10.680  -1.823  1.00  0.00      BrD ATOM    762  CA   TYR   47      -7.033
12.587  -2.097  1.00  0.00      BrD ATOM    763  HA   TYR   47      -6.102
12.042  -2.050  1.00  0.00      BrD ATOM    764  CB   TYR   47      -7.099
13.345  -3.424  1.00  0.00      BrD ATOM    765  HB1  TYR   47      -7.889
14.080  -3.370  1.00  0.00      BrD ATOM    766  HB2  TYR   47      -6.158
13.848  -3.590  1.00  0.00      BrD ATOM    767  CG   TYR   47      -7.370
12.459  -4.619  1.00  0.00      BrD ATOM    768  CD1  TYR   47      -8.056
12.946  -5.725  1.00  0.00      BrD ATOM    769  HD1  TYR   47      -8.397
13.971  -5.722  1.00  0.00      BrD ATOM    770  CD2  TYR   47      -6.940
11.137  -4.644  1.00  0.00      BrD ATOM    771  HD2  TYR   47      -6.405
10.742  -3.792  1.00  0.00      BrD ATOM    772  CE1  TYR   47      -8.306
12.143  -6.821  1.00  0.00      BrD ATOM    773  HE1  TYR   47      -8.841
12.540  -7.671  1.00  0.00      BrD ATOM    774  CE2  TYR   47      -7.186
10.328  -6.738  1.00  0.00      BrD ATOM    775  HE2  TYR   47      -6.845
9.303  -5.739  1.00  0.00      BrD ATOM    776  CZ   TYR   47      -7.870
10.835  -6.823  1.00  0.00      BrD ATOM    777  OH   TYR   47      -8.117
10.032  -7.912  1.00  0.00      BrD ATOM    778  HH   TYR   47      -7.572
10.317  -8.650  1.00  0.00      BrD ATOM    779  C    TYR   47      -7.065
13.572  -0.933  1.00  0.00      BrD ATOM    780  O    TYR   47      -6.183
13.605  -0.095  1.00  0.00      BrD ATOM    781  N    GLU   48      -8.144
14.376  -0.887  1.00  0.00      BrD ATOM    782  HN   GLU   48      -8.830
14.304  -1.584  1.00  0.00      BrD ATOM    783  CA   GLU   48      -6.309
15.365   0.174  1.00  0.00      BrD ATOM    784  HA   GLU   48      -7.569
16.138   0.024  1.00  0.00      BrD ATOM    785  CB   GLU   48      -5.704
15.991   0.104  1.00  0.00      BrD ATOM    786  HB1  GLU   48      -5.746
16.827   0.786  1.00  0.00      BrD ATOM    787  HB2  GLU   48      -6.432
15.254   0.408  1.00  0.00      BrD ATOM    788  CG   GLU   48      -4.079
16.488  -1.283  1.00  0.00      BrD ATOM    789  HG1  GLU   48      -3.268
17.086  -1.669  1.00  0.00      BrD ATOM    790  HG2  GLU   48      -4.335
15.635  -1.927  1.00  0.00      BrD ATOM    791  CD   GLU   48      -3.341
17.328  -1.282  1.00  0.00      BrD ATOM    792  OE1  GLU   48      -2.059
17.320  -0.260  1.00  0.00      BrD ATOM    793  OE2  GLU   48      -1.612
17.994  -2.304  1.00  0.00      BrD ATOM    794  C    GLU   48      -8.091
14.736   1.547  1.00  0.00      BrD ATOM    795  O    GLU   48      -7.683
15.410   2.493  1.00  0.00      BrD ATOM    796  N    VAL   49      -8.360
13.439   1.645  1.00  0.00      BrD ATOM    797  HN   VAL   49      -8.682
12.958   0.854  1.00  0.00      BrD ATOM    798  CA   VAL   49      -8.192
12.712   2.899  1.00  0.00      BrD ATOM    799  HA   VAL   49      -7.919
13.423   3.665  1.00  0.00      BrD ATOM    800  CB   VAL   49      -9.495
12.010   3.332  1.00  0.00      BrD ATOM    801  HB   VAL   49      -9.555
11.064   2.815  1.00  0.00      BrD ATOM    802  CG1  VAL   49     -10.713
12.834   2.949  1.00  0.00      BrD ATOM    803  HG11 VAL   49     -11.006
12.591   1.937  1.00  0.00      BrD ATOM    804  HG12 VAL   49     -10.472
13.884   3.011  1.00  0.00      BrD ATOM    805  HG13 VAL   49     -11.526
12.609   3.622  1.00  0.00      BrD ATOM    806  CG2  VAL   49      -9.475
11.729   4.827  1.00  0.00      BrD ATOM    807  HG21 VAL   49      -9.393
12.661   5.367  1.00  0.00      BrD ATOM    808  HG22 VAL   49      -8.628
11.101   5.062  1.00  0.00      BrD ATOM    809  HG23 VAL   49     -10.387
11.226   5.111  1.00  0.00      BrD ATOM    810  C    VAL   49      -7.100
11.656   2.787  1.00  0.00      BrD ATOM    811  O    VAL   49      -6.592
11.167   3.797  1.00  0.00      BrD ATOM    812  N    ILE   50      -6.763
11.281   1.558  1.00  0.00      BrD ATOM    813  HN   ILE   50      -7.214
11.686   0.792  1.00  0.00      BrD ATOM    814  CA   ILE   50      -5.769
10.245   1.324  1.00  0.00      BrD ATOM    815  HA   ILE   50      -5.842
9.783   2.274  1.00  0.00      BrD ATOM    816  CB   ILE   50      -6.291
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9.152   0.366  1.00  0.00      BrD ATOM    817  HB  ILE    50      -6.001
9.428  -0.635  1.00  0.00      BrD ATOM    818  CG1 ILE    50      -7.818
9.035   0.436  1.00  0.00      BrD ATOM    819 HG11 ILE    50      -8.256
10.011  0.288  1.00  0.00      BrD ATOM    820 HG12 ILE    50      -8.158
8.371  -0.344  1.00  0.00      BrD ATOM    821  CG2 ILE    50      -5.644
7.815   0.684  1.00  0.00      BrD ATOM    822 HG21 ILE    50      -5.490
7.264  -0.233  1.00  0.00      BrD ATOM    823 HG22 ILE    50      -6.289
7.250   1.339  1.00  0.00      BrD ATOM    824 HG23 ILE    50      -4.694
7.981   1.169  1.00  0.00      BrD ATOM    825  CD1 ILE    50      -8.324
8.489   1.757  1.00  0.00      BrD ATOM    826 HD11 ILE    50      -8.330
9.293   2.489  1.00  0.00      BrD ATOM    827 HD12 ILE    50      -7.674
7.704   2.094  1.00  0.00      BrD ATOM    828 HD13 ILE    50      -9.326
8.116   1.631  1.00  0.00      BrD ATOM    829  C   ILE    50      -4.490
10.827  0.738  1.00  0.00      BrD ATOM    830  O   ILE    50      -4.504
11.444 -0.327  1.00  0.00      BrD ATOM    831  N   ARG    51      -3.384
10.597  1.428  1.00  0.00      BrD ATOM    832  HN  ARG    51      -3.443
10.086  2.260  1.00  0.00      BrD ATOM    833  CA  ARG    51      -2.082
11.061  0.969  1.00  0.00      BrD ATOM    834  HA  ARG    51      -2.068
12.139  1.024  1.00  0.00      BrD ATOM    835  CB  ARG    51      -0.988
10.491  1.870  1.00  0.00      BrD ATOM    836  HB1 ARG    51      -1.452
10.081  2.754  1.00  0.00      BrD ATOM    837  HB2 ARG    51      -0.478
9.698   1.361  1.00  0.00      BrD ATOM    838  CG  ARG    51      0.048
11.516  2.301  1.00  0.00      BrD ATOM    839  HG1 ARG    51      -0.399
12.185  3.022  1.00  0.00      BrD ATOM    840  HG2 ARG    51      0.883
11.000  2.753  1.00  0.00      BrD ATOM    841  CD  ARG    51      0.552
12.329  1.120  1.00  0.00      BrD ATOM    842  HD1 ARG    51      0.514
11.713  0.233  1.00  0.00      BrD ATOM    843  HD2 ARG    51      -0.090
13.187  0.989  1.00  0.00      BrD ATOM    844  NE  ARG    51      1.923
12.789  1.318  1.00  0.00      BrD ATOM    845  HE  ARG    51      2.296
12.730  2.222  1.00  0.00      BrD ATOM    846  CZ  ARG    51      2.683
13.279  0.344  1.00  0.00      BrD ATOM    847  NH1 ARG    51      3.921
13.678  0.602  1.00  0.00      BrD ATOM    848 HH11 ARG    51      4.491
14.046 -0.132  1.00  0.00      BrD ATOM    849 HH12 ARG    51      4.284
13.610  1.532  1.00  0.00      BrD ATOM    850  NH2 ARG    51      2.206
13.371 -0.890  1.00  0.00      BrD ATOM    851 HH21 ARG    51      2.779
13.739 -1.622  1.00  0.00      BrD ATOM    852 HH22 ARG    51      1.273
13.071 -1.089  1.00  0.00      BrD ATOM    853  C   ARG    51      -1.836
10.631 -0.471  1.00  0.00      BrD ATOM    854  O   ARG    51      -1.644
11.461 -1.360  1.00  0.00      BrD ATOM    855  N   SER    52      -1.843
9.322  -0.687  1.00  0.00      BrD ATOM    856  HN  SER    52      -2.010
8.718   0.067  1.00  0.00      BrD ATOM    857  CA  SER    52      -1.634
8.753  -2.012  1.00  0.00      BrD ATOM    858  HA  SER    52      -1.991
9.462  -2.740  1.00  0.00      BrD ATOM    859  CB  SER    52      -0.145
8.497  -2.253  1.00  0.00      BrD ATOM    860  HB1 SER    52      0.426
8.900  -1.430  1.00  0.00      BrD ATOM    861  HB2 SER    52      0.028
7.433  -2.325  1.00  0.00      BrD ATOM    862  OG  SER    52      0.290
9.112  -3.453  1.00  0.00      BrD ATOM    863  HG  SER    52      -0.218
8.768  -4.192  1.00  0.00      BrD ATOM    864  C   SER    52      -2.415
7.450  -2.148  1.00  0.00      BrD ATOM    865  O   SER    52      -1.912
6.382  -1.801  1.00  0.00      BrD ATOM    866  N   PRO    53      -3.675
7.518  -2.619  1.00  0.00      BrD ATOM    867  CA  PRO    53      -4.531
6.344  -2.745  1.00  0.00      BrD ATOM    868  HA  PRO    53      -4.993
6.101  -1.800  1.00  0.00      BrD ATOM    869  CB  PRO    53      -5.620
6.776  -3.738  1.00  0.00      BrD ATOM    870  HB1 PRO    53      -5.555
6.173  -4.630  1.00  0.00      BrD ATOM    871  HB2 PRO    53      -6.590
6.638  -3.284  1.00  0.00      BrD ATOM    872  CG  PRO    53      -5.171
8.224  -4.043  1.00  0.00      BrD ATOM    873  HG1 PRO    53      -6.296
8.775  -3.959  1.00  0.00      BrD ATOM    874  HG2 PRO    53      -4.969
8.321  -5.041  1.00  0.00      BrD ATOM    875  CD  PRO    53      -4.177
8.735  -3.034  1.00  0.00      BrD ATOM    876  HD1 PRO    53      -4.886
9.191  -2.200  1.00  0.00      BrD ATOM    877  HD2 PRO    53      -3.704
9.437  -3.498  1.00  0.00      BrD ATOM    878  C   PRO    53      -3.770
5.120  -3.252  1.00  0.00      BrD ATOM    879  O   PRO    53      -3.456
4.218  -2.475  1.00  0.00      BrD ATOM    880  N   MET    54      -3.471
5.089  -4.553  1.00  0.00      BrD ATOM    881  HN  MET    54      -3.738
5.838  -5.124  1.00  0.00      BrD ATOM    882  CA  MET    54      -2.734
3.970  -5.149  1.00  0.00      BrD ATOM    883  HA  MET    54      -2.905
3.995  -6.215  1.00  0.00      BrD ATOM    884  CB  MET    54      -1.236
4.127  -4.877  1.00  0.00      BrD ATOM    885  HB1 MET    54      -0.936
5.129  -5.145  1.00  0.00      BrD ATOM    886  HB2 MET    54      -1.057
3.978  -3.822  1.00  0.00      BrD ATOM    887  CG  MET    54      -0.368
3.147  -5.649  1.00  0.00      BrD ATOM    888  HG1 MET    54      -0.510
2.160  -5.235  1.00  0.00      BrD ATOM    889  HG2 MET    54      0.666
3.438  -5.537  1.00  0.00      BrD ATOM    890  SD  MET    54      -0.767
3.101  -7.407  1.00  0.00      BrD ATOM    891  CE  MET    54      -2.176
1.995  -7.401  1.00  0.00      BrD ATOM    892  HE1 MET    54      -2.086
1.294  -8.214  1.00  0.00      BrD ATOM    893  HE2 MET    54      -3.085
2.567  -7.518  1.00  0.00      BrD ATOM    894  HE3 MET    54      -2.208
1.457  -6.465  1.00  0.00      BrD ATOM    895  C   MET    54      -3.229
2.630  -4.602  1.00  0.00      BrD ATOM    896  O   MET    54      -2.556
1.990  -3.795  1.00  0.00      BrD ATOM    897  N   ASP    55      -4.422
2.232  -5.029  1.00  0.00      BrD ATOM    898  HN  ASP    55      -4.919
2.803  -5.652  1.00  0.00      BrD ATOM    899  CA  ASP    55      -5.045
1.005  -4.544  1.00  0.00      BrD ATOM    900  HA  ASP    55      -5.234
1.142  -3.490  1.00  0.00      BrD ATOM    901  CB  ASP    55      -6.391
0.793  -5.249  1.00  0.00      BrD ATOM    902  HB1 ASP    55      -6.327
0.045  -5.917  1.00  0.00      BrD ATOM    903  HB2 ASP    55      -6.631
1.679  -5.817  1.00  0.00      BrD ATOM    904  CG  ASP    55      -7.520
0.526  -4.269  1.00  0.00      BrD ATOM    905  OD1 ASP    55      -8.426
0.256  -4.602  1.00  0.00      BrD ATOM    906  OD2 ASP    55      -7.496
1.126  -3.169  1.00  0.00      BrD ATOM    907  C   ASP    55      -4.121
0.212  -4.704  1.00  0.00      BrD ATOM    908  O   ASP    55      -3.406
0.670  -3.772  1.00  0.00      BrD ATOM    909  N   LEU    56      -4.142
0.856  -5.870  1.00  0.00      BrD ATOM    910  HN  LEU    56      -4.715

0.533  -6.586  1.00  0.00      BrD ATOM    911  CA  LEU    56      -3.306
2.030  -6.111  1.00  0.00      BrD ATOM    912  HA  LEU    56      -2.301
1.790  -5.810  1.00  0.00      BrD ATOM    913  CB  LEU    56      -3.804
3.224  -5.292  1.00  0.00      BrD ATOM    914  HB1 LEU    56      -3.692
4.115  -5.892  1.00  0.00      BrD ATOM    915  HB2 LEU    56      -4.852
3.082  -5.089  1.00  0.00      BrD ATOM    916  CG  LEU    56      -3.088
3.451  -3.962  1.00  0.00      BrD ATOM    917  HG  LEU    56      -3.356
2.661  -3.279  1.00  0.00      BrD ATOM    918  CD1 LEU    56      -3.521
4.770  -3.344  1.00  0.00      BrD ATOM    919 HD11 LEU    56      -2.809
5.539  -3.606  1.00  0.00      BrD ATOM    920 HD12 LEU    56      -4.497
5.040  -3.719  1.00  0.00      BrD ATOM    921 HD13 LEU    56      -3.562
4.668  -2.270  1.00  0.00      BrD ATOM    922  CD2 LEU    56      -1.580
3.419  -4.153  1.00  0.00      BrD ATOM    923 HD21 LEU    56      -1.352
3.388  -5.209  1.00  0.00      BrD ATOM    924 HD22 LEU    56      -1.144
4.306  -3.716  1.00  0.00      BrD ATOM    925 HD23 LEU    56      -1.175
2.542  -3.671  1.00  0.00      BrD ATOM    926  C   LEU    56      -3.305
2.400  -7.587  1.00  0.00      BrD ATOM    927  O   LEU    56      -2.271
2.760  -8.150  1.00  0.00      BrD ATOM    928  N   LYS    57      -4.475
2.304  -8.207  1.00  0.00      BrD ATOM    929  HN  LYS    57      -5.261
2.020  -7.696  1.00  0.00      BrD ATOM    930  CA  LYS    57      -4.634
2.639  -9.615  1.00  0.00      BrD ATOM    931  HA  LYS    57      -4.577
3.712  -9.704  1.00  0.00      BrD ATOM    932  CB  LYS    57      -6.007
2.179 -10.108  1.00  0.00      BrD ATOM    933  HB1 LYS    57      -6.765
2.764  -9.608  1.00  0.00      BrD ATOM    934  HB2 LYS    57      -6.139
1.139  -9.850  1.00  0.00      BrD ATOM    935  CG  LYS    57      -6.203
2.328 -11.608  1.00  0.00      BrD ATOM    936  HG1 LYS    57      -5.383
1.845 -12.118  1.00  0.00      BrD ATOM    937  HG2 LYS    57      -7.132
1.856 -11.889  1.00  0.00      BrD ATOM    938  CD  LYS    57      -6.248
3.790 -12.024  1.00  0.00      BrD ATOM    939  HD1 LYS    57      -6.259
4.098 -12.327  1.00  0.00      BrD ATOM    940  HD2 LYS    57      -6.671
4.383 -11.181  1.00  0.00      BrD ATOM    941  CE  LYS    57      -7.210
4.011 -13.180  1.00  0.00      BrD ATOM    942  HE1 LYS    57      -7.354
3.073 -13.697  1.00  0.00      BrD ATOM    943  HE2 LYS    57      -6.778
4.732 -13.858  1.00  0.00      BrD ATOM    944  NZ  LYS    57      -8.532
4.515 -12.715  1.00  0.00      BrD ATOM    945  HZ1 LYS    57      -8.403
5.182 -11.926  1.00  0.00      BrD ATOM    946  HZ2 LYS    57      -9.022
5.003 -13.492  1.00  0.00      BrD ATOM    947  HZ3 LYS    57      -9.122
3.723 -12.391  1.00  0.00      BrD ATOM    948  C   LYS    57      -3.533
2.015 -10.473  1.00  0.00      BrD ATOM    949  O   LYS    57      -3.222
2.816 -11.553  1.00  0.00      BrD ATOM    950  N   THR    58      -2.941
0.923  -9.989  1.00  0.00      BrD ATOM    951  HN  THR    58      -3.240
0.552  -9.135  1.00  0.00      BrD ATOM    952  CA  THR    58      -1.901
0.230 -10.742  1.00  0.00      BrD ATOM    953  HA  THR    58      -1.819
0.717 -11.702  1.00  0.00      BrD ATOM    954  CB  THR    58      -2.307
1.233 -10.967  1.00  0.00      BrD ATOM    955  HB  THR    58      -2.611
1.660 -10.024  1.00  0.00      BrD ATOM    956  OG1 THR    58      -3.403
1.313 -11.862  1.00  0.00      BrD ATOM    957  HG1 THR    58      -3.101
1.133 -12.755  1.00  0.00      BrD ATOM    958  CG2 THR    58      -1.197
2.099 -11.525  1.00  0.00      BrD ATOM    959 HG21 THR    58      -0.808
2.734 -10.743  1.00  0.00      BrD ATOM    960 HG22 THR    58      -1.585
2.710 -12.326  1.00  0.00      BrD ATOM    961 HG23 THR    58      -0.405
1.469 -11.904  1.00  0.00      BrD ATOM    962  C   THR    58      -0.539
0.305 -10.045  1.00  0.00      BrD ATOM    963  O   THR    58      0.499
0.220 -10.701  1.00  0.00      BrD ATOM    964  N   MET    59      -0.537
0.445  -8.721  1.00  0.00      BrD ATOM    965  HN  MET    59      -1.388
0.503  -8.238  1.00  0.00      BrD ATOM    966  CA  MET    59      0.716
0.505  -7.972  1.00  0.00      BrD ATOM    967  HA  MET    59      1.401
0.191  -8.436  1.00  0.00      BrD ATOM    968  CB  MET    59      0.499
0.070  -6.513  1.00  0.00      BrD ATOM    969  HB1 MET    59      1.430
0.316  -6.125  1.00  0.00      BrD ATOM    970  HB2 MET    59      -0.238
0.717  -6.498  1.00  0.00      BrD ATOM    971  CG  MET    59      0.022
1.176  -5.583  1.00  0.00      BrD ATOM    972  HG1 MET    59      -0.822
0.811  -5.017  1.00  0.00      BrD ATOM    973  HG2 MET    59      -0.286
2.022  -6.180  1.00  0.00      BrD ATOM    974  SD  MET    59      1.300
1.715  -4.431  1.00  0.00      BrD ATOM    975  CE  MET    59      1.463
0.259  -3.400  1.00  0.00      BrD ATOM    976  HE1 MET    59      0.629
0.205  -2.715  1.00  0.00      BrD ATOM    977  HE2 MET    59      1.474
0.624  -4.022  1.00  0.00      BrD ATOM    978  HE3 MET    59      2.386
0.316  -2.841  1.00  0.00      BrD ATOM    979  C   MET    59      1.345
1.901  -8.036  1.00  0.00      BrD ATOM    980  O   MET    59      2.535
2.067  -7.767  1.00  0.00      BrD ATOM    981  N   SER    60      0.542
2.898  -8.392  1.00  0.00      BrD ATOM    982  HN  SER    60      -0.399
2.710  -8.590  1.00  0.00      BrD ATOM    983  CA  SER    60      1.025
4.271  -8.478  1.00  0.00      BrD ATOM    984  HA  SER    60      1.685
4.442  -7.640  1.00  0.00      BrD ATOM    985  CB  SER    60      -0.147
5.250  -8.396  1.00  0.00      BrD ATOM    986  HB1 SER    60      -0.610
5.171  -7.424  1.00  0.00      BrD ATOM    987  HB2 SER    60      -0.871
5.006  -9.159  1.00  0.00      BrD ATOM    988  OG  SER    60      0.286
6.585  -8.588  1.00  0.00      BrD ATOM    989  HG  SER    60      -0.145
6.953  -9.361  1.00  0.00      BrD ATOM    990  C   SER    60      1.803
4.503  -9.770  1.00  0.00      BrD ATOM    991  O   SER    60      2.636
5.405  -9.850  1.00  0.00      BrD ATOM    992  N   GLU    61      1.519
3.690 -10.782  1.00  0.00      BrD ATOM    993  HN  GLU    61      0.819
2.998 -10.661  1.00  0.00      BrD ATOM    994  CA  GLU    61      2.182
3.820 -12.075  1.00  0.00      BrD ATOM    995  HA  GLU    61      2.295
4.874 -12.283  1.00  0.00      BrD ATOM    996  CB  GLU    61      1.326
3.187 -13.174  1.00  0.00      BrD ATOM    997  HB1 GLU    61      1.820
3.324 -14.125  1.00  0.00      BrD ATOM    998  HB2 GLU    61      1.232
2.129 -12.977  1.00  0.00      BrD ATOM    999  CG  GLU    61      -0.071
3.779 -13.274  1.00  0.00      BrD ATOM   1000  HG1 GLU    61      -0.494
3.836 -12.282  1.00  0.00      BrD ATOM   1001  HG2 GLU    61      -0.679
3.132 -13.889  1.00  0.00      BrD ATOM   1002  CD  GLU    61      -0.071
5.167 -13.803  1.00  0.00      BrD ATOM   1003  OE1 GLU    61      -1.024
5.488 -14.427  1.00  0.00      BrD ATOM   1004  OE2 GLU    61      0.876

5.934 -11.617  1.00  0.00      BrD ATOM   1005  C   GLU    61      3.565
3.174 -12.060  1.00  0.00      BrD ATOM   1006  O   GLU    61      4.466
3.601 -12.782  1.00  0.00      BrD ATOM   1007  N   ARG    62      3.726
2.137 -11.244  1.00  0.00      BrD ATOM   1008  HN  ARG    62      2.971
1.836 -10.697  1.00  0.00      BrD ATOM   1009  CA  ARG    62      4.999
1.428 -11.155  1.00  0.00      BrD ATOM   1010  HA  ARG    62      5.352
1.262 -12.162  1.00  0.00      BrD ATOM   1011  CB  ARG    62      4.807
0.075 -10.468  1.00  0.00      BrD ATOM   1012  HB1 ARG    62      5.753
0.241 -10.052  1.00  0.00      BrD ATOM   1013  HB2 ARG    62      4.091
0.167  -9.668  1.00  0.00      BrD ATOM   1014  CG  ARG    62      4.312
1.018 -11.404  1.00  0.00      BrD ATOM   1015  HG1 ARG    62      4.852
1.928 -11.195  1.00  0.00      BrD ATOM   1016  HG2 ARG    62      4.494
0.714 -12.424  1.00  0.00      BrD ATOM   1017  CD  ARG    62      2.826
1.278 -11.225  1.00  0.00      BrD ATOM   1018  HD1 ARG    62      2.484
0.738 -10.356  1.00  0.00      BrD ATOM   1019  HD2 ARG    62      2.675
2.336 -11.072  1.00  0.00      BrD ATOM   1020  NE  ARG    62      2.052
0.851 -12.387  1.00  0.00      BrD ATOM   1021  HE  ARG    62      1.621
0.028 -12.346  1.00  0.00      BrD ATOM   1022  CZ  ARG    62      1.903
1.585 -13.685  1.00  0.00      BrD ATOM   1023 NH1 ARG    62      1.183
1.125 -14.498  1.00  0.00      BrD ATOM   1024 HH11 ARG    62      1.072
1.678 -15.324  1.00  0.00      BrD ATOM   1025 HH12 ARG    62      0.752
0.224 -14.437  1.00  0.00      BrD ATOM   1026 NH2 ARG    62      2.673
2.780 -13.571  1.00  0.00      BrD ATOM   1027 HH21 ARG    62      2.359
3.329 -14.399  1.00  0.00      BrD ATOM   1028 HH22 ARG    62      3.018
3.130 -12.809  1.00  0.00      BrD ATOM   1029  C   ARG    62      6.040
2.255 -10.405  1.00  0.00      BrD ATOM   1030  O   ARG    62      7.101
2.569 -10.945  1.00  0.00      BrD ATOM   1031  N   LEU    63      5.734
2.606  -9.158  1.00  0.00      BrD ATOM   1032  HN  LEU    63      6.875
2.326  -8.780  1.00  0.00      BrD ATOM   1033  CA  LEU    63      6.651
3.396  -8.339  1.00  0.00      BrD ATOM   1034  HA  LEU    63      7.496
2.771  -8.093  1.00  0.00      BrD ATOM   1035  CB  LEU    63      5.962
3.840  -7.043  1.00  0.00      BrD ATOM   1036  HB1 LEU    63      5.009
4.277  -7.302  1.00  0.00      BrD ATOM   1037  HB2 LEU    63      5.780
2.962  -6.442  1.00  0.00      BrD ATOM   1038  CG  LEU    63      6.726
4.857  -6.186  1.00  0.00      BrD ATOM   1039  HG  LEU    63      6.629
4.754  -5.156  1.00  0.00      BrD ATOM   1040  CD1 LEU    63      8.237
4.605  -6.247  1.00  0.00      BrD ATOM   1041 HD11 LEU    63      8.420
3.584  -6.547  1.00  0.00      BrD ATOM   1042 HD12 LEU    63      8.685
5.277  -6.965  1.00  0.00      BrD ATOM   1043 HD13 LEU    63      8.671
4.779  -5.273  1.00  0.00      BrD ATOM   1044  CD2 LEU    63      6.414
6.277  -6.627  1.00  0.00      BrD ATOM   1045 HD21 LEU    63      7.332
6.804  -6.842  1.00  0.00      BrD ATOM   1046 HD22 LEU    63      5.798
6.248  -7.514  1.00  0.00      BrD ATOM   1047 HD23 LEU    63      5.883
6.787  -5.836  1.00  0.00      BrD ATOM   1048  C   LEU    63      7.150
4.618  -9.103  1.00  0.00      BrD ATOM   1049  O   LEU    63      8.354
4.853  -9.203  1.00  0.00      BrD ATOM   1050  N   LYS    64      6.214
5.390  -9.643  1.00  0.00      BrD ATOM   1051  HN  LYS    64      5.271
5.150  -9.525  1.00  0.00      BrD ATOM   1052  CA  LYS    64      6.551
6.592 -10.397  1.00  0.00      BrD ATOM   1053  HA  LYS    64      6.929
7.325  -9.699  1.00  0.00      BrD ATOM   1054  CB  LYS    64      5.303
7.152 -11.082  1.00  0.00      BrD ATOM   1055  HB1 LYS    64      4.649
6.332 -11.340  1.00  0.00      BrD ATOM   1056  HB2 LYS    64      5.602
7.661 -11.987  1.00  0.00      BrD ATOM   1057  CG  LYS    64      4.523
8.131 -10.221  1.00  0.00      BrD ATOM   1058  HG1 LYS    64      3.533
7.724 -10.047  1.00  0.00      BrD ATOM   1059  HG2 LYS    64      5.035
8.254  -9.278  1.00  0.00      BrD ATOM   1060  CD  LYS    64      4.398
9.488 -10.894  1.00  0.00      BrD ATOM   1061  HD1 LYS    64      3.343
9.798 -10.870  1.00  0.00      BrD ATOM   1062  HD2 LYS    64      4.726
9.402 -11.920  1.00  0.00      BrD ATOM   1063  CE  LYS    64      5.243
10.538 -10.192  1.00  0.00      BrD ATOM   1064  HE1 LYS    64      5.904
10.043  -9.496  1.00  0.00      BrD ATOM   1065  HE2 LYS    64      4.589
11.207  -9.653  1.00  0.00      BrD ATOM   1066  NZ  LYS    64      6.060
11.330 -11.154  1.00  0.00      BrD ATOM   1067  HZ1 LYS    64      6.712
11.955 -10.638  1.00  0.00      BrD ATOM   1068  HZ2 LYS    64      6.615
10.693 -11.761  1.00  0.00      BrD ATOM   1069  HZ3 LYS    64      5.441
11.911 -11.754  1.00  0.00      BrD ATOM   1070  C   LYS    64      7.629
6.305 -11.439  1.00  0.00      BrD ATOM   1071  O   LYS    64      8.376
7.200 -11.834  1.00  0.00      BrD ATOM   1072  N   ASN    65      7.705
5.052 -11.880  1.00  0.00      BrD ATOM   1073  HN  ASN    65      7.080
4.383 -11.531  1.00  0.00      BrD ATOM   1074  CA  ASN    65      8.688
4.657 -12.883  1.00  0.00      BrD ATOM   1075  HA  ASN    65      9.212
5.547 -13.198  1.00  0.00      BrD ATOM   1076  CB  ASN    65      7.989
4.034 -14.092  1.00  0.00      BrD ATOM   1077  HB1 ASN    65      8.680
3.376 -14.600  1.00  0.00      BrD ATOM   1078  HB2 ASN    65      7.137
3.463 -13.754  1.00  0.00      BrD ATOM   1079  CG  ASN    65      7.506
5.076 -15.081  1.00  0.00      BrD ATOM   1080  OD1 ASN    65      8.177
6.080 -15.320  1.00  0.00      BrD ATOM   1081  ND2 ASN    65      6.334
4.844 -15.660  1.00  0.00      BrD ATOM   1082 HD21 ASN    65      5.854
4.024 -15.421  1.00  0.00      BrD ATOM   1083 HD22 ASN    65      5.997
5.502 -16.301  1.00  0.00      BrD ATOM   1084  C   ASN    65      9.703
3.677 -12.308  1.00  0.00      BrD ATOM   1085  O   ASN    65      10.237
2.829 -13.023  1.00  0.00      BrD ATOM   1086  N   ARG    66      9.973
3.804 -11.014  1.00  0.00      BrD ATOM   1087  HN  ARG    66      9.523
4.505 -10.498  1.00  0.00      BrD ATOM   1088  CA  ARG    66      10.942
2.963 -10.346  1.00  0.00      BrD ATOM   1089  HA  ARG    66      10.826
3.082  -9.281  1.00  0.00      BrD ATOM   1090  CB  ARG    66      12.357
3.347 -10.739  1.00  0.00      BrD ATOM   1091  HB1 ARG    66      12.323
3.875 -11.680  1.00  0.00      BrD ATOM   1092  HB2 ARG    66      12.959
2.458 -10.854  1.00  0.00      BrD ATOM   1093  CG  ARG    66      13.016
4.243  -9.713  1.00  0.00      BrD ATOM   1094  HG1 ARG    66      13.744
3.666  -9.163  1.00  0.00      BrD ATOM   1095  HG2 ARG    66      12.262
4.613  -9.038  1.00  0.00      BrD ATOM   1096  CD  ARG    66      11.710
5.423 -10.388  1.00  0.00      BrD ATOM   1097  HD1 ARG    66      11.483
5.439 -11.416  1.00  0.00      BrD ATOM   1098  HD2 ARG    66      11.398
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6.329  -9.898  1.00  0.00      BrD ATOM   1099  NE  ARG    66      15.162  -
5.351 -10.237  1.00  0.00      BrD ATOM   1100  HE  ARG    66      15.688  -
5.256 -11.059  1.00  0.00      BrD ATOM   1101  CZ  ARG    66      15.801  -
5.407  -9.074  1.00  0.00      BrD ATOM   1102 NH1  ARG    66      15.117  -
5.536  -7.945  1.00  0.00      BrD ATOM   1103 HH11 ARG    66      15.599  -
5.578  -7.070  1.00  0.00      BrD ATOM   1104 HH12 ARG    66      14.118  -
5.591  -7.969  1.00  0.00      BrD ATOM   1105 NH2  ARG    66      17.125  -
5.334  -9.037  1.00  0.00      BrD ATOM   1106 HH21 ARG    66      17.604  -
5.377  -8.161  1.00  0.00      BrD ATOM   1107 HH22 ARG    66      17.643  -
5.237  -9.887  1.00  0.00      BrD ATOM   1108  C   ARG    66      10.708  -
1.474 -10.682  1.00  0.00      BrD ATOM   1109  O   ARG    66      11.654  -
0.705 -10.850  1.00  0.00      BrD ATOM   1110  N   TYR    67       9.441  -
1.097 -10.781  1.00  0.00      BrD ATOM   1111  HN  TYR    67       8.736  -
1.759 -10.633  1.00  0.00      BrD ATOM   1112  CA  TYR    67       9.075
0.280 -11.094  1.00  0.00      BrD ATOM   1113  HA  TYR    67       9.952
0.780 -11.472  1.00  0.00      BrD ATOM   1114  CB  TYR    67       7.982
0.309 -12.164  1.00  0.00      BrD ATOM   1115 HB1  TYR    67       7.062  -
0.061 -11.738  1.00  0.00      BrD ATOM   1116 HB2  TYR    67       8.276  -
0.330 -12.984  1.00  0.00      BrD ATOM   1117  CG  TYR    67       7.713
1.687 -12.723  1.00  0.00      BrD ATOM   1118 CD1  TYR    67       7.042
2.639 -11.970  1.00  0.00      BrD ATOM   1119 HD1  TYR    67       6.718
3.385 -10.973  1.00  0.00      BrD ATOM   1120 CD2  TYR    67       8.122
2.032 -14.005  1.00  0.00      BrD ATOM   1121 HD2  TYR    67       8.645
1.301 -14.604  1.00  0.00      BrD ATOM   1122 CE1  TYR    67       6.787
3.899 -12.475  1.00  0.00      BrD ATOM   1123 HE1  TYR    67       6.261
4.625 -11.872  1.00  0.00      BrD ATOM   1124 CE2  TYR    67       7.872
3.291 -14.518  1.00  0.00      BrD ATOM   1125 HE2  TYR    67       8.198
3.541 -15.516  1.00  0.00      BrD ATOM   1126  CZ  TYR    67       7.204
4.220 -13.749  1.00  0.00      BrD ATOM   1127  OH  TYR    67       6.953
5.475 -14.256  1.00  0.00      BrD ATOM   1128  HH  TYR    67       7.446
6.127 -13.753  1.00  0.00      BrD ATOM   1129  C   TYR    67       8.606
1.006  -9.840  1.00  0.00      BrD ATOM   1130  O   TYR    67       8.910
2.181  -9.639  1.00  0.00      BrD ATOM   1131  N   TYR    68       7.880
0.291  -8.990  1.00  0.00      BrD ATOM   1132  HN  TYR    68       7.686  -
0.647  -9.197  1.00  0.00      BrD ATOM   1133  CA  TYR    68       7.401
0.855  -7.736  1.00  0.00      BrD ATOM   1134  HA  TYR    68       7.528
1.924  -7.788  1.00  0.00      BrD ATOM   1135  CB  TYR    68       5.918
0.531  -7.538  1.00  0.00      BrD ATOM   1136 HB1  TYR    68       5.646  -
0.286  -8.188  1.00  0.00      BrD ATOM   1137 HB2  TYR    68       5.758
0.234  -6.512  1.00  0.00      BrD ATOM   1138  CG  TYR    68       4.987
1.689  -7.033  1.00  0.00      BrD ATOM   1139 CD1  TYR    68       5.378
2.734  -8.664  1.00  0.00      BrD ATOM   1140 ND1  TYR    68       6.364
2.717  -9.101  1.00  0.00      BrD ATOM   1141 CD2  TYR    68       3.712
1.732  -7.283  1.00  0.00      BrD ATOM   1142 HD2  TYR    68       3.392
0.927  -6.638  1.00  0.00      BrD ATOM   1143 CE1  TYR    68       4.526
3.788  -8.933  1.00  0.00      BrD ATOM   1144 HE1  TYR    68       4.849
4.591  -9.579  1.00  0.00      BrD ATOM   1145 CE2  TYR    68       2.655
2.782  -7.549  1.00  0.00      BrD ATOM   1146 HE2  TYR    68       1.868
2.797  -7.110  1.00  0.00      BrD ATOM   1147  CZ  TYR    68       3.267
3.807  -8.374  1.00  0.00      BrD ATOM   1148  OH  TYR    68       2.416
4.855  -8.639  1.00  0.00      BrD ATOM   1149  HH  TYR    68       2.457
5.490  -7.920  1.00  0.00      BrD ATOM   1150  C   TYR    68       8.206
0.327  -6.548  1.00  0.00      BrD ATOM   1151  O   TYR    68       8.001
0.759  -5.416  1.00  0.00      BrD ATOM   1152  N   VAL    69       9.149  -
0.579  -6.816  1.00  0.00      BrD ATOM   1153  HN  VAL    69       9.268  -
0.888  -7.735  1.00  0.00      BrD ATOM   1154  CA  VAL    69       9.977  -
1.170  -5.769  1.00  0.00      BrD ATOM   1155  HA  VAL    69       9.397  -
1.941  -5.285  1.00  0.00      BrD ATOM   1156  CB  VAL    69      11.232  -
1.825  -6.366  1.00  0.00      BrD ATOM   1157  HB  VAL    69      10.922  -
2.537  -7.117  1.00  0.00      BrD ATOM   1158 CG1  VAL    69      12.107  -
0.778  -7.032  1.00  0.00      BrD ATOM   1159 HG11 VAL    69      11.701  -
0.536  -8.003  1.00  0.00      BrD ATOM   1160 HG12 VAL    69      13.108  -
1.165  -7.146  1.00  0.00      BrD ATOM   1161 HG13 VAL    69      12.131
0.111  -6.420  1.00  0.00      BrD ATOM   1162 CG2  VAL    69      12.001  -
2.572  -5.291  1.00  0.00      BrD ATOM   1163 HG21 VAL    69      11.389  -
3.370  -4.899  1.00  0.00      BrD ATOM   1164 HG22 VAL    69      12.256  -
1.889  -4.494  1.00  0.00      BrD ATOM   1165 HG23 VAL    69      12.904  -
2.985  -5.716  1.00  0.00      BrD ATOM   1166  C   VAL    69      10.409  -
0.149  -4.717  1.00  0.00      BrD ATOM   1167  O   VAL    69      10.642  -
0.506  -3.565  1.00  0.00      BrD ATOM   1168  N   SER    70      10.508
1.123  -5.110  1.00  0.00      BrD ATOM   1169  HN  SER    70      10.321
1.350  -6.044  1.00  0.00      BrD ATOM   1170  CA  SER    70      10.909
2.190  -4.189  1.00  0.00      BrD ATOM   1171  HA  SER    70      11.983
2.146  -4.081  1.00  0.00      BrD ATOM   1172  CB  SER    70      10.525
3.552  -4.767  1.00  0.00      BrD ATOM   1173 HB1  SER    70      11.246
3.838  -5.518  1.00  0.00      BrD ATOM   1174 HB2  SER    70       9.546
3.483  -5.216  1.00  0.00      BrD ATOM   1175  OG  SER    70      10.498
4.547  -3.758  1.00  0.00      BrD ATOM   1176  HG  SER    70      10.908
5.349  -4.088  1.00  0.00      BrD ATOM   1177  C   SER    70      10.268
2.011  -2.610  1.00  0.00      BrD ATOM   1178  O   SER    70       9.252
1.330  -2.674  1.00  0.00      BrD ATOM   1179  N   LYS    71      10.881
2.605  -1.791  1.00  0.00      BrD ATOM   1180  HN  LYS    71      11.708
3.118  -1.958  1.00  0.00      BrD ATOM   1181  CA  LYS    71      10.393
2.470  -0.422  1.00  0.00      BrD ATOM   1182  HA  LYS    71      10.268
1.418  -0.226  1.00  0.00      BrD ATOM   1183  CB  LYS    71      11.419
3.036   0.564  1.00  0.00      BrD ATOM   1184 HB1  LYS    71      10.915
3.287   1.485  1.00  0.00      BrD ATOM   1185 HB2  LYS    71      11.848
2.933   0.142  1.00  0.00      BrD ATOM   1186  CG  LYS    71      12.550
2.074   0.888  1.00  0.00      BrD ATOM   1187 HG1  LYS    71      13.359
2.237   0.191  1.00  0.00      BrD ATOM   1188 HG2  LYS    71      12.188
1.061   0.791  1.00  0.00      BrD ATOM   1189  CD  LYS    71      13.069
2.279   3.302  1.00  0.00      BrD ATOM   1190 HD1  LYS    71      12.295
2.001   3.002  1.00  0.00      BrD ATOM   1191 HD2  LYS    71      13.936
1.652   2.452  1.00  0.00      BrD ATOM   1192  CE  LYS    71      13.460
3.727   2.548  1.00  0.00      BrD ATOM   1193 HE1  LYS    71      14.024
4.086   1.699  1.00  0.00      BrD ATOM   1194 HE2  LYS    71      12.561
4.316   2.655  1.00  0.00      BrD ATOM   1195  NZ  LYS    71      14.287
3.879   3.777  1.00  0.00      BrD ATOM   1196 HZ1  LYS    71      13.870
3.334   4.558  1.00  0.00      BrD ATOM   1197 HZ2  LYS    71      14.334
4.880   4.055  1.00  0.00      BrD ATOM   1198 HZ3  LYS    71      15.252
3.531   3.604  1.00  0.00      BrD ATOM   1199  C   LYS    71       9.041
3.160  -0.231  1.00  0.00      BrD ATOM   1200  O   LYS    71       7.992
2.529  -0.362  1.00  0.00      BrD ATOM   1201  N   LYS    72       9.070
4.447   0.109  1.00  0.00      BrD ATOM   1202  HN  LYS    72       9.933
4.898   0.211  1.00  0.00      BrD ATOM   1203  CA  LYS    72       7.844
5.201   0.351  1.00  0.00      BrD ATOM   1204  HA  LYS    72       7.196
4.818   1.255  1.00  0.00      BrD ATOM   1205  CB  LYS    72       8.167
6.684   0.547  1.00  0.00      BrD ATOM   1206 HB1  LYS    72       7.269
7.216   0.752  1.00  0.00      BrD ATOM   1207 HB2  LYS    72       8.601
7.070  -0.364  1.00  0.00      BrD ATOM   1208  CG  LYS    72       9.136
6.950   1.687  1.00  0.00      BrD ATOM   1209 HG1  LYS    72       9.870
6.158   1.715  1.00  0.00      BrD ATOM   1210 HG2  LYS    72       9.629
7.895   1.515  1.00  0.00      BrD ATOM   1211  CD  LYS    72       8.419
7.004   3.027  1.00  0.00      BrD ATOM   1212 HD1  LYS    72       7.831
6.104   3.147  1.00  0.00      BrD ATOM   1213 HD2  LYS    72       9.155
7.065   3.816  1.00  0.00      BrD ATOM   1214  CE  LYS    72       7.497
8.208   3.117  1.00  0.00      BrD ATOM   1215 HE1  LYS    72       7.708  -
8.869   2.288  1.00  0.00      BrD ATOM   1216 HE2  LYS    72       6.474
7.868   3.054  1.00  0.00      BrD ATOM   1217  NZ  LYS    72       7.681
8.956   4.391  1.00  0.00      BrD ATOM   1218 HZ1  LYS    72       8.150
8.352   5.096  1.00  0.00      BrD ATOM   1219 HZ2  LYS    72       6.758
9.256   4.766  1.00  0.00      BrD ATOM   1220 HZ3  LYS    72       8.267
9.800   4.229  1.00  0.00      BrD ATOM   1221  C   LYS    72       6.052
5.034  -0.794  1.00  0.00      BrD ATOM   1222  O   LYS    72       5.641
5.001  -0.578  1.00  0.00      BrD ATOM   1223  N   LEU    73       7.170
4.933  -2.011  1.00  0.00      BrD ATOM   1224  HN  LEU    73       8.143
4.972  -2.121  1.00  0.00      BrD ATOM   1225  CA  LEU    73       6.528
4.786  -3.191  1.00  0.00      BrD ATOM   1226  HA  LEU    73       5.982
5.708  -3.323  1.00  0.00      BrD ATOM   1227  CB  LEU    73       7.394
4.539  -4.427  1.00  0.00      BrD ATOM   1228 HB1  LEU    73       7.447
3.474  -4.596  1.00  0.00      BrD ATOM   1229 HB2  LEU    73       8.389
4.903  -4.219  1.00  0.00      BrD ATOM   1230  CG  LEU    73       6.896
5.206  -5.711  1.00  0.00      BrD ATOM   1231  HG  LEU    73       5.937
4.787  -5.978  1.00  0.00      BrD ATOM   1232 CD1  LEU    73       7.860
4.943  -6.857  1.00  0.00      BrD ATOM   1233 HD11 LEU    73       8.166
3.907  -6.840  1.00  0.00      BrD ATOM   1234 HD12 LEU    73       8.729
5.576  -6.750  1.00  0.00      BrD ATOM   1235 HD13 LEU    73       7.372
5.158  -7.796  1.00  0.00      BrD ATOM   1236 CD2  LEU    73       6.710
6.701  -5.498  1.00  0.00      BrD ATOM   1237 HD21 LEU    73       7.104
6.979  -4.531  1.00  0.00      BrD ATOM   1238 HD22 LEU    73       5.659
6.943  -5.541  1.00  0.00      BrD ATOM   1239 HD23 LEU    73       7.237
7.243  -6.270  1.00  0.00      BrD ATOM   1240  C   LEU    73       5.528
3.645  -3.025  1.00  0.00      BrD ATOM   1241  O   LEU    73       4.318
3.660  -3.061  1.00  0.00      BrD ATOM   1242  N   PHE    74       6.041
2.432  -2.860  1.00  0.00      BrD ATOM   1243  HN  PHE    74       7.014
2.323  -2.855  1.00  0.00      BrD ATOM   1244  CA  PHE    74       5.192
1.283  -2.721  1.00  0.00      BrD ATOM   1245  HA  PHE    74       4.364
1.359  -3.406  1.00  0.00      BrD ATOM   1246  CB  PHE    74       5.984  -
0.003  -3.084  1.00  0.00      BrD ATOM   1247 HB1  PHE    74       6.730  -
0.181  -2.324  1.00  0.00      BrD ATOM   1248 HB2  PHE    74       6.473
0.154  -4.030  1.00  0.00      BrD ATOM   1249  CG  PHE    74       5.141  -
1.240  -3.202  1.00  0.00      BrD ATOM   1250 CD1  PHE    74       4.952  -
1.851  -4.431  1.00  0.00      BrD ATOM   1251 HD1  PHE    74       5.412  -
1.425  -5.311  1.00  0.00      BrD ATOM   1252 CD2  PHE    74       4.546  -
1.797  -2.082  1.00  0.00      BrD ATOM   1253 HD2  PHE    74       4.691  -
1.332  -1.118  1.00  0.00      BrD ATOM   1254 CE1  PHE    74       4.181  -
2.993  -4.542  1.00  0.00      BrD ATOM   1255 HE1  PHE    74       4.039  -
3.458  -5.506  1.00  0.00      BrD ATOM   1256 CE2  PHE    74       3.780  -
2.942  -2.186  1.00  0.00      BrD ATOM   1257 HE2  PHE    74       3.315  -
3.362  -1.304  1.00  0.00      BrD ATOM   1258  CZ  PHE    74       3.593  -
3.538  -3.418  1.00  0.00      BrD ATOM   1259  HZ  PHE    74       2.989  -
4.430  -3.502  1.00  0.00      BrD ATOM   1260  C   PHE    74       4.643
1.116  -1.305  1.00  0.00      BrD ATOM   1261  O   PHE    74       3.503
0.694  -1.111  1.00  0.00      BrD ATOM   1262  N   MET    75       5.466
1.447  -0.318  1.00  0.00      BrD ATOM   1263  HN  MET    75       6.372
1.755  -0.532  1.00  0.00      BrD ATOM   1264  CA  MET    75       5.072
1.308   1.078  1.00  0.00      BrD ATOM   1265  HA  MET    75       4.603
0.339   1.187  1.00  0.00      BrD ATOM   1266  CB  MET    75       6.300
1.365   1.984  1.00  0.00      BrD ATOM   1267 HB1  MET    75       6.001
1.734   2.954  1.00  0.00      BrD ATOM   1268 HB2  MET    75       7.021
2.043   1.554  1.00  0.00      BrD ATOM   1269  CG  MET    75       6.966
0.014   2.171  1.00  0.00      BrD ATOM   1270 HG1  MET    75       7.524
0.029   3.092  1.00  0.00      BrD ATOM   1271 HG2  MET    75       6.200  -
0.744   2.231  1.00  0.00      BrD ATOM   1272  SD  MET    75       8.086  -
0.403   0.822  1.00  0.00      BrD ATOM   1273  CE  MET    75       8.173  -
2.182   1.002  1.00  0.00      BrD ATOM   1274 HE1  MET    75       7.211  -
2.557   1.319  1.00  0.00      BrD ATOM   1275 HE2  MET    75       8.917  -
2.435   1.741  1.00  0.00      BrD ATOM   1276 HE3  MET    75       8.438  -
2.630   0.054  1.00  0.00      BrD ATOM   1277  C   MET    75       4.067
2.374   1.496  1.00  0.00      BrD ATOM   1278  O   MET    75       2.939
2.052   1.866  1.00  0.00      BrD ATOM   1279  N   ALA    76       4.472
3.642   1.462  1.00  0.00      BrD ATOM   1280  HN  ALA    76       5.380
3.854   1.163  1.00  0.00      BrD ATOM   1281  CA  ALA    76       3.573
4.722   1.861  1.00  0.00      BrD ATOM   1282  HA  ALA    76       3.409
4.638   2.922  1.00  0.00      BrD ATOM   1283  CB  ALA    76       4.182
6.083   1.595  1.00  0.00      BrD ATOM   1284 HB1  ALA    76       4.234
6.252   0.931  1.00  0.00      BrD ATOM   1285 HB2  ALA    76       5.172
6.125   2.021  1.00  0.00      BrD ATOM   1286 HB3  ALA    76       3.558
6.842   3.049  1.00  0.00      BrD ATOM   1287  C   ALA    76       2.240
4.601   1.147  1.00  0.00      BrD ATOM   1288  O   ALA    76       1.211
5.026   1.666  1.00  0.00      BrD ATOM   1289  N   ASP    77       3.270
4.014  -0.044  1.00  0.00      BrD ATOM   1290  HN  ASP    77       3.124
3.685  -0.294  1.00  0.00      BrD ATOM   1291  CA  ASP    77       1.058
3.804  -0.818  1.00  0.00      BrD ATOM   1292  HA  ASP    77       0.460
4.701  -0.750  1.00  0.00      BrD ATOM   1293  CB  ASP    77       1.392
3.834  -2.281  1.00  0.00      BrD ATOM   1294 HB1  ASP    77       2.196
2.817  -2.334  1.00  0.00      BrD ATOM   1295 HB2  ASP    77       0.521
3.128  -2.776  1.00  0.00      BrD ATOM   1296  CG  ASP    77       1.817
4.790  -3.018  1.00  0.00      BrD ATOM   1297 OD1  ASP    77       1.253
4.995  -4.159  1.00  0.00      BrD ATOM   1298 OD2  ASP    77       2.613
5.569  -2.453  1.00  0.00      BrD ATOM   1299  C   ASP    77       0.268
2.641  -0.243  1.00  0.00      BrD ATOM   1300  O   ASP    77      -0.950
2.717  -0.113  1.00  0.00      BrD ATOM   1301  N   LEU    78       0.970
1.569   0.119  1.00  0.00      BrD ATOM   1302  HN  LEU    78       1.944
1.570   0.006  1.00  0.00      BrD ATOM   1303  CA  LEU    78       0.319
0.411   0.711  1.00  0.00      BrD ATOM   1304  HA  LEU    78      -0.493
0.122   0.060  1.00  0.00      BrD ATOM   1305  CB  LEU    78       1.280  -
0.761   0.849  1.00  0.00      BrD ATOM   1306 HB1  LEU    78       2.212  -
0.516   0.358  1.00  0.00      BrD ATOM   1307 HB2  LEU    78       1.480  -
0.922   1.900  1.00  0.00      BrD ATOM   1308  CG  LEU    78       0.736  -
2.052   0.259  1.00  0.00      BrD ATOM   1309  HG  LEU    78      -0.336  -
2.023   0.293  1.00  0.00      BrD ATOM   1310 CD1  LEU    78       1.143  -
3.189  -1.193  1.00  0.00      BrD ATOM   1311 HD11 LEU    78       1.413  -
3.213  -1.398  1.00  0.00      BrD ATOM   1312 HD12 LEU    78       1.985  -
1.543  -1.388  1.00  0.00      BrD ATOM   1313 HD13 LEU    78       0.317  -
1.901  -1.625  1.00  0.00      BrD ATOM   1314 CD2  LEU    78       1.189  -
3.236   1.078  1.00  0.00      BrD ATOM   1315 HD21 LEU    78       2.264  -
3.266   1.099  1.00  0.00      BrD ATOM   1316 HD22 LEU    78       0.808  -
4.145   0.640  1.00  0.00      BrD ATOM   1317 HD23 LEU    78       0.809  -
3.130   2.084  1.00  0.00      BrD ATOM   1318  C   LEU    78      -0.283
0.769   2.066  1.00  0.00      BrD ATOM   1319  O   LEU    78      -1.459
0.663   2.292  1.00  0.00      BrD ATOM   1320  N   GLN    79       0.611
1.252   2.952  1.00  0.00      BrD ATOM   1321  HN  GLN    79       1.551
1.353   2.700  1.00  0.00      BrD ATOM   1322  CA  GLN    79       0.171
1.723   4.254  1.00  0.00      BrD ATOM   1323  HA  GLN    79      -0.198
0.873   4.807  1.00  0.00      BrD ATOM   1324  CB  GLN    79       1.338
2.361   5.015  1.00  0.00      BrD ATOM   1325 HB1  GLN    79       1.045
2.520   6.038  1.00  0.00      BrD ATOM   1326 HB2  GLN    79       2.180
1.686   4.991  1.00  0.00      BrD ATOM   1327  CG  GLN    79       1.781
3.694   4.448  1.00  0.00      BrD ATOM   1328 HG1  GLN    79       1.501
3.740   3.407  1.00  0.00      BrD ATOM   1329 HG2  GLN    79       2.855
3.766   4.536  1.00  0.00      BrD ATOM   1330  CD  GLN    79       1.158
4.871   5.172  1.00  0.00      BrD ATOM   1331 OE1  GLN    79       0.409
5.651   4.585  1.00  0.00      BrD ATOM   1332 NE2  GLN    79       1.467
5.005   6.457  1.00  0.00      BrD ATOM   1333 HE21 GLN    79       1.079
5.757   6.950  1.00  0.00      BrD ATOM   1334 HE22 GLN    79       2.070
4.346   6.859  1.00  0.00      BrD ATOM   1335  C   GLN    79      -0.960
2.732   4.074  1.00  0.00      BrD ATOM   1336  O   GLN    79      -1.787
2.924   4.964  1.00  0.00      BrD ATOM   1337  N   ARG    80      -0.997
3.356   2.895  1.00  0.00      BrD ATOM   1338  HN  ARG    80      -0.321
3.140   2.216  1.00  0.00      BrD ATOM   1339  CA  ARG    80      -2.048
4.306   2.560  1.00  0.00      BrD ATOM   1340  HA  ARG    80      -2.276
4.880   3.447  1.00  0.00      BrD ATOM   1341  CB  ARG    80      -1.579
5.253   1.455  1.00  0.00      BrD ATOM   1342 HB1  ARG    80      -2.401
5.429   0.773  1.00  0.00      BrD ATOM   1343 HB2  ARG    80      -0.770
4.785   0.908  1.00  0.00      BrD ATOM   1344  CG  ARG    80      -1.092
6.598   1.964  1.00  0.00      BrD ATOM   1345 HG1  ARG    80      -0.290
6.434   2.669  1.00  0.00      BrD ATOM   1346 HG2  ARG    80      -0.728
7.180   1.131  1.00  0.00      BrD ATOM   1347  CD  ARG    80      -2.206
7.367   2.654  1.00  0.00      BrD ATOM   1348 HD1  ARG    80      -3.054
6.711   2.780  1.00  0.00      BrD ATOM   1349 HD2  ARG    80      -2.486
8.203   2.031  1.00  0.00      BrD ATOM   1350  NE  ARG    80      -1.796
7.867   1.962  1.00  0.00      BrD ATOM   1351  HE  ARG    80      -0.837
7.674   4.166  1.00  0.00      BrD ATOM   1352  CZ  ARG    80      -2.648
8.310   4.881  1.00  0.00      BrD ATOM   1353 NH1  ARG    80      -2.198
8.750   6.047  1.00  0.00      BrD ATOM   1354 HH11 ARG    80      -1.216
8.749   6.237  1.00  0.00      BrD ATOM   1355 HH12 ARG    80      -2.840
9.083   6.738  1.00  0.00      BrD ATOM   1356 NH2  ARG    80      -3.950
8.314   4.633  1.00  0.00      BrD ATOM   1357 HH21 ARG    80      -4.590
8.647   5.326  1.00  0.00      BrD ATOM   1358 HH22 ARG    80      -4.293
7.983   3.754  1.00  0.00      BrD ATOM   1359  C   ARG    80      -3.305
3.568   2.114  1.00  0.00      BrD ATOM   1360  O   ARG    80      -4.417
3.922   2.502  1.00  0.00      BrD ATOM   1361  N   VAL    81      -3.116
2.536   1.293  1.00  0.00      BrD ATOM   1362  HN  VAL    81      -2.203
2.301   1.024  1.00  0.00      BrD ATOM   1363  CA  VAL    81      -4.231
1.738   0.799  1.00  0.00      BrD ATOM   1364  HA  VAL    81      -4.849
2.374   0.182  1.00  0.00      BrD ATOM   1365  CB  VAL    81      -3.742
0.556  -0.063  1.00  0.00      BrD ATOM   1366  HB  VAL    81      -3.104  -
0.068   0.546  1.00  0.00      BrD ATOM   1367 CG1  VAL    81      -2.926
1.057  -1.244  1.00  0.00      BrD ATOM   1368 HG11 VAL    81      -3.462
0.861  -2.159  1.00  0.00      BrD ATOM   1369 HG12 VAL    81      -1.973
0.545  -1.268  1.00  0.00      BrD ATOM   1370 HG13 VAL    81      -2.763
2.119  -1.146  1.00  0.00      BrD ATOM   1371 CG2  VAL    81      -4.916  -
0.287  -0.539  1.00  0.00      BrD ATOM   1372 HG21 VAL    81      -4.851  -
0.425  -1.608  1.00  0.00      BrD ATOM   1373 HG22 VAL    81      -5.841
0.215  -0.297  1.00  0.00      BrD ATOM   1374 HG23 VAL    81      -4.890  -
1.250  -0.050  1.00  0.00      BrD ATOM   1375  C   VAL    81      -5.069
1.206   1.957  1.00  0.00      BrD ATOM   1376  O   VAL    81      -6.293
1.339   1.964  1.00  0.00      BrD ATOM   1377  N   PHE    82      -4.400
0.610   2.937  1.00  0.00      BrD ATOM   1378  HN  PHE    82      -3.424
0.540   2.876  1.00  0.00      BrD ATOM   1379  CA  PHE    82      -5.079
0.070   4.108  1.00  0.00      BrD ATOM   1380  HA  PHE    82      -5.919  -
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0.514   3.764  1.00  0.00      BrD ATOM   1381  CB  PHE    82      -4.131  -
0.833   4.899  1.00  0.00      BrD ATOM   1382  HB1 PHE    82      -3.486  -
0.220   5.511  1.00  0.00      BrD ATOM   1383  HB2 PHE    82      -4.712  -
1.484   5.536  1.00  0.00      BrD ATOM   1384  CG  PHE    82      -3.261  -
1.695   4.028  1.00  0.00      BrD ATOM   1385  CD1 PHE    82      -1.979  -
2.035   4.426  1.00  0.00      BrD ATOM   1386  HD1 PHE    82      -1.606  -
1.677   5.376  1.00  0.00      BrD ATOM   1387  CD2 PHE    82      -3.725  -
2.162   2.809  1.00  0.00      BrD ATOM   1388  HD2 PHE    82      -4.723  -
1.901   2.487  1.00  0.00      BrD ATOM   1389  CE1 PHE    82      -1.177  -
2.827   3.628  1.00  0.00      BrD ATOM   1390  HE1 PHE    82      -0.179  -
3.046   3.951  1.00  0.00      BrD ATOM   1391  CE2 PHE    82      -2.928  -
2.952   2.004  1.00  0.00      BrD ATOM   1392  HE2 PHE    82      -3.302  -
3.311   1.057  1.00  0.00      BrD ATOM   1393  CZ  PHE    82      -1.651  -
3.284   2.413  1.00  0.00      BrD ATOM   1394  HZ  PHE    82      -1.029  -
3.906   1.769  1.00  0.00      BrD ATOM   1395  C   PHE    82      -8.594
1.197   4.994  1.00  0.00      BrD ATOM   1396  O   PHE    82      -6.745
1.180   5.431  1.00  0.00      BrD ATOM   1397  N   THR    83      -4.740
2.185   5.241  1.00  0.00      BrD ATOM   1398  HN  THR    83      -3.841
2.149   4.852  1.00  0.00      BrD ATOM   1399  CA  THR    83      -5.119
3.337   6.048  1.00  0.00      BrD ATOM   1400  HA  THR    83      -5.437
2.977   7.019  1.00  0.00      BrD ATOM   1401  CB  THR    83      -3.927
4.282   6.216  1.00  0.00      BrD ATOM   1402  HB  THR    83      -3.525
4.516   5.240  1.00  0.00      BrD ATOM   1403  OG1 THR    83      -2.905
3.666   6.982  1.00  0.00      BrD ATOM   1404  HG1 THR    83      -3.138
3.699   7.913  1.00  0.00      BrD ATOM   1405  CG2 THR    83      -4.283
5.589   6.892  1.00  0.00      BrD ATOM   1406 HG21 THR    83      -4.813
6.222   6.196  1.00  0.00      BrD ATOM   1407 HG22 THR    83      -3.379
6.085   7.214  1.00  0.00      BrD ATOM   1408 HG23 THR    83      -4.910
5.391   7.749  1.00  0.00      BrD ATOM   1409  C   THR    83      -6.286
4.077   5.402  1.00  0.00      BrD ATOM   1410  O   THR    83      -7.073
4.735   6.082  1.00  0.00      BrD ATOM   1411  N   ASN    84      -6.391
3.956   4.082  1.00  0.00      BrD ATOM   1412  HN  ASN    84      -5.732
3.418   3.597  1.00  0.00      BrD ATOM   1413  CA  ASN    84      -7.458
4.609   3.334  1.00  0.00      BrD ATOM   1414  HA  ASN    84      -7.546
5.622   3.698  1.00  0.00      BrD ATOM   1415  CB  ASN    84      -7.113
4.640   1.844  1.00  0.00      BrD ATOM   1416  HB1 ASN    84      -7.095
3.629   1.464  1.00  0.00      BrD ATOM   1417  HB2 ASN    84      -6.138
5.086   1.716  1.00  0.00      BrD ATOM   1418  CG  ASN    84      -8.115
5.438   1.035  1.00  0.00      BrD ATOM   1419  OD1 ASN    84      -9.269
5.596   1.433  1.00  0.00      BrD ATOM   1420  ND2 ASN    84      -7.677
5.945  -0.111  1.00  0.00      BrD ATOM   1421 HD21 ASN    84      -6.745
5.778  -0.365  1.00  0.00      BrD ATOM   1422 HD22 ASN    84      -8.302
6.465  -0.655  1.00  0.00      BrD ATOM   1423  C   ASN    84      -8.788
3.893   3.544  1.00  0.00      BrD ATOM   1424  O   ASN    84      -9.745
4.477   4.051  1.00  0.00      BrD ATOM   1425  N   CYS    85      -8.842
2.623   3.150  1.00  0.00      BrD ATOM   1426  HN  CYS    85      -8.046
2.213   2.751  1.00  0.00      BrD ATOM   1427  CA  CYS    85     -10.058
1.827   3.291  1.00  0.00      BrD ATOM   1428  HA  CYS    85     -10.778
2.193   2.575  1.00  0.00      BrD ATOM   1429  CB  CYS    85      -9.765
0.354   2.995  1.00  0.00      BrD ATOM   1430  HB1 CYS    85      -8.806
0.277   2.504  1.00  0.00      BrD ATOM   1431  HB2 CYS    85      -9.732  -
0.193   3.926  1.00  0.00      BrD ATOM   1432  SG  CYS    85     -10.992  -
0.444   1.933  1.00  0.00      BrD ATOM   1433  HG  CYS    85     -10.844  -
0.144   1.033  1.00  0.00      BrD ATOM   1434  C   CYS    85     -10.645
1.965   4.692  1.00  0.00      BrD ATOM   1435  O   CYS    85     -11.842
2.203   4.854  1.00  0.00      BrD ATOM   1436  N   LYS    86      -9.794
1.817   5.701  1.00  0.00      BrD ATOM   1437  HN  LYS    86      -8.852
1.626   5.508  1.00  0.00      BrD ATOM   1438  HA  LYS    86     -10.228
1.921   7.089  1.00  0.00      BrD ATOM   1439  HA  LYS    86     -11.111
1.310   7.203  1.00  0.00      BrD ATOM   1440  CB  LYS    86      -9.137
1.395   8.023  1.00  0.00      BrD ATOM   1441  HB1 LYS    86      -9.063
0.325   7.903  1.00  0.00      BrD ATOM   1442  HB2 LYS    86      -9.416
1.616   9.043  1.00  0.00      BrD ATOM   1443  CG  LYS    86      -7.768
1.998   7.763  1.00  0.00      BrD ATOM   1444  HG1 LYS    86      -7.809
2.583   6.857  1.00  0.00      BrD ATOM   1445  HG2 LYS    86      -7.050
1.199   7.645  1.00  0.00      BrD ATOM   1446  CD  LYS    86      -7.325
2.892   8.910  1.00  0.00      BrD ATOM   1447  HD1 LYS    86      -6.477
3.478   8.590  1.00  0.00      BrD ATOM   1448  HD2 LYS    86      -8.140
3.548   9.177  1.00  0.00      BrD ATOM   1449  CE  LYS    86      -6.929
2.076  10.130  1.00  0.00      BrD ATOM   1450  HE1 LYS    86      -7.418
1.114  10.078  1.00  0.00      BrD ATOM   1451  HE2 LYS    86      -5.858
1.935  10.120  1.00  0.00      BrD ATOM   1452  NZ  LYS    86      -7.317
2.749  11.400  1.00  0.00      BrD ATOM   1453  HZ1 LYS    86      -6.019
2.174  11.909  1.00  0.00      BrD ATOM   1454  HZ2 LYS    86      -7.729
3.682  11.199  1.00  0.00      BrD ATOM   1455  HZ3 LYS    86      -6.482
2.874  12.008  1.00  0.00      BrD ATOM   1456  C   LYS    86     -10.579
3.360   7.456  1.00  0.00      BrD ATOM   1457  O   LYS    86     -11.293
3.603   8.429  1.00  0.00      BrD ATOM   1458  N   GLU    87     -10.076
4.314   6.676  1.00  0.00      BrD ATOM   1459  HN  GLU    87      -9.514
4.066   5.914  1.00  0.00      BrD ATOM   1460  CA  GLU    87     -10.380
5.724   6.926  1.00  0.00      BrD ATOM   1461  HA  GLU    87     -10.510
5.848   7.986  1.00  0.00      BrD ATOM   1462  CB  GLU    87      -9.158
6.583   6.498  1.00  0.00      BrD ATOM   1463  HB1 GLU    87      -9.513
7.572   6.249  1.00  0.00      BrD ATOM   1464  HB2 GLU    87      -8.706
6.141   5.622  1.00  0.00      BrD ATOM   1465  CG  GLU    87      -8.088
6.716   7.570  1.00  0.00      BrD ATOM   1466  HG1 GLU    87      -7.954
5.757   8.048  1.00  0.00      BrD ATOM   1467  HG2 GLU    87      -7.163
7.016   7.101  1.00  0.00      BrD ATOM   1468  CD  GLU    87      -8.446
7.740   8.629  1.00  0.00      BrD ATOM   1469  OE1 GLU    87      -9.092
8.751   8.283  1.00  0.00      BrD ATOM   1470  OE2 GLU    87      -8.079
7.531   9.805  1.00  0.00      BrD ATOM   1471  C   GLU    87     -11.604
6.172   6.183  1.00  0.00      BrD ATOM   1472  O   GLU    87     -12.542
6.692   6.787  1.00  0.00      BrD ATOM   1473  N   TYR    88     -11.617
5.962   4.871  1.00  0.00      BrD ATOM   1474  HN  TYR    88     -10.840

5.561   4.446  1.00  0.00      BrD ATOM   1475  CA  TYR    88     -12.759
6.339   4.046  1.00  0.00      BrD ATOM   1476  HA  TYR    88     -13.070
7.330   4.344  1.00  0.00      BrD ATOM   1477  CB  TYR    88     -12.361
6.363   2.568  1.00  0.00      BrD ATOM   1478  HB1 TYR    88     -11.310
6.602   2.489  1.00  0.00      BrD ATOM   1479  HB2 TYR    88     -12.537
5.388   2.139  1.00  0.00      BrD ATOM   1480  CG  TYR    88     -13.128
7.376   1.748  1.00  0.00      BrD ATOM   1481  CD1 TYR    88     -12.606
8.640   1.505  1.00  0.00      BrD ATOM   1482  HD1 TYR    88     -11.639
8.096   1.914  1.00  0.00      BrD ATOM   1483  CD2 TYR    88     -14.372
7.066   1.213  1.00  0.00      BrD ATOM   1484  HD2 TYR    88     -14.792
6.087   1.392  1.00  0.00      BrD ATOM   1485  CE1 TYR    88     -13.302
9.568   0.755  1.00  0.00      BrD ATOM   1486  HE1 TYR    88     -12.880
10.546   0.578  1.00  0.00     BrD ATOM   1487  CE2 TYR    88     -15.075
7.989   0.462  1.00  0.00      BrD ATOM   1488  HE2 TYR    88     -16.042
7.730   0.055  1.00  0.00      BrD ATOM   1489  CZ  TYR    88     -14.526
9.238   0.236  1.00  0.00      BrD ATOM   1490  OH  TYR    88     -15.233
10.159  -0.512  1.00  0.00     BrD ATOM   1491  HH  TYR    88     -15.995
10.465  -0.014  1.00  0.00     BrD ATOM   1492  C   TYR    88     -13.923
5.374   4.256  1.00  0.00      BrD ATOM   1493  O   TYR    88     -14.369
4.711   3.320  1.00  0.00      BrD ATOM   1494  N   ASN    89     -14.408
5.298   5.492  1.00  0.00      BrD ATOM   1495  HN  ASN    89     -14.012
5.852   6.195  1.00  0.00      BrD ATOM   1496  CA  ASN    89     -15.518
4.414   5.827  1.00  0.00      BrD ATOM   1497  HA  ASN    89     -16.355
4.336   4.958  1.00  0.00      BrD ATOM   1498  CB  ASN    89     -14.996
3.023   6.192  1.00  0.00      BrD ATOM   1499  HB1 ASN    89     -15.816
2.421   6.557  1.00  0.00      BrD ATOM   1500  HB2 ASN    89     -14.578
2.559   5.311  1.00  0.00      BrD ATOM   1501  CG  ASN    89     -13.925
3.072   7.263  1.00  0.00      BrD ATOM   1502  OD1 ASN    89     -13.552
4.147   7.734  1.00  0.00      BrD ATOM   1503  ND2 ASN    89     -13.424
1.904   7.655  1.00  0.00      BrD ATOM   1504 HD21 ASN    89     -13.770
1.090   7.236  1.00  0.00      BrD ATOM   1505 HD22 ASN    89     -12.731
1.909   8.367  1.00  0.00      BrD ATOM   1506  C   ASN    89     -16.332
4.982   6.985  1.00  0.00      BrD ATOM   1507  O   ASN    89     -16.088
4.658   8.167  1.00  0.00      BrD ATOM   1508  N   ALA    90     -17.296
5.836   6.659  1.00  0.00      BrD ATOM   1509  HN  ALA    90     -17.438
6.058   5.715  1.00  0.00      BrD ATOM   1510  CA  ALA    90     -18.142
6.458   7.670  1.00  0.00      BrD ATOM   1511  HA  ALA    90     -17.525
7.122   8.258  1.00  0.00      BrD ATOM   1512  CB  ALA    90     -19.228
7.291   7.006  1.00  0.00      BrD ATOM   1513  HB1 ALA    90     -19.280
7.045   5.956  1.00  0.00      BrD ATOM   1514  HB2 ALA    90     -18.997
8.340   7.119  1.00  0.00      BrD ATOM   1515  HB3 ALA    90     -20.179
7.081   7.473  1.00  0.00      BrD ATOM   1516  C   ALA    90     -18.764
5.414   8.594  1.00  0.00      BrD ATOM   1517  O   ALA    90     -18.728
5.557   9.817  1.00  0.00      BrD ATOM   1518  N   PRO    91     -19.346
4.347   8.021  1.00  0.00      BrD ATOM   1519  CA  PRO    91     -20.000
3.290   8.783  1.00  0.00      BrD ATOM   1520  HA  PRO    91     -20.495
3.681   9.659  1.00  0.00      BrD ATOM   1521  CB  PRO    91     -21.048
2.740   7.800  1.00  0.00      BrD ATOM   1522  HB1 PRO    91     -20.932
1.670   7.715  1.00  0.00      BrD ATOM   1523  HB2 PRO    91     -22.038
2.966   8.169  1.00  0.00      BrD ATOM   1524  CG  PRO    91     -20.794
3.419   6.483  1.00  0.00      BrD ATOM   1525  HG1 PRO    91     -20.778
2.684   5.692  1.00  0.00      BrD ATOM   1526  HG2 PRO    91     -21.566
4.151   6.296  1.00  0.00      BrD ATOM   1527  CD  PRO    91     -19.456
4.095   6.587  1.00  0.00      BrD ATOM   1528  HD1 PRO    91     -18.670
3.436   6.247  1.00  0.00      BrD ATOM   1529  HD2 PRO    91     -19.450
5.018   6.027  1.00  0.00      BrD ATOM   1530  C   PRO    91     -19.035
2.183   9.196  1.00  0.00      BrD ATOM   1531  O   PRO    91     -19.458
1.079   9.540  1.00  0.00      BrD ATOM   1532  N   GLU    92     -17.736
2.481   9.160  1.00  0.00      BrD ATOM   1533  HN  GLU    92     -17.462
3.377   8.873  1.00  0.00      BrD ATOM   1534  CA  GLU    92     -16.703
1.506   9.521  1.00  0.00      BrD ATOM   1535  HA  GLU    92     -15.779
1.838   9.083  1.00  0.00      BrD ATOM   1536  CB  GLU    92     -16.529
1.439  11.039  1.00  0.00      BrD ATOM   1537  HB1 GLU    92     -15.786
0.690  11.272  1.00  0.00      BrD ATOM   1538  HB2 GLU    92     -16.182
2.399  11.393  1.00  0.00      BrD ATOM   1539  CG  GLU    92     -17.805
1.092  11.778  1.00  0.00      BrD ATOM   1540  HG1 GLU    92     -18.550
1.831  11.537  1.00  0.00      BrD ATOM   1541  HG2 GLU    92     -18.143
0.119  11.452  1.00  0.00      BrD ATOM   1542  CD  GLU    92     -17.622
1.062  13.283  1.00  0.00      BrD ATOM   1543  OE1 GLU    92     -18.536
1.517  14.001  1.00  0.00      BrD ATOM   1544  OE2 GLU    92     -16.564
0.581  13.743  1.00  0.00      BrD ATOM   1545  C   GLU    92     -17.029
0.119   8.974  1.00  0.00      BrD ATOM   1546  O   GLU    92     -16.862  -
0.887   9.663  1.00  0.00      BrD ATOM   1547  N   SER    93     -17.508
0.081   7.736  1.00  0.00      BrD ATOM   1548  HN  SER    93     -17.420
0.919   7.240  1.00  0.00      BrD ATOM   1549  CA  SER    93     -17.863  -
1.176   7.092  1.00  0.00      BrD ATOM   1550  HA  SER    93     -18.677  -
1.616   7.649  1.00  0.00      BrD ATOM   1551  CB  SER    93     -18.317  -
0.925   5.653  1.00  0.00      BrD ATOM   1552  HB1 SER    93     -17.475  -
1.052   4.986  1.00  0.00      BrD ATOM   1553  HB2 SER    93     -18.695
0.084   5.568  1.00  0.00      BrD ATOM   1554  OG  SER    93     -19.339  -
1.830   5.274  1.00  0.00      BrD ATOM   1555  HG  SER    93     -19.610  -
1.648   4.371  1.00  0.00      BrD ATOM   1556  C   SER    93     -16.686  -
2.141   7.099  1.00  0.00      BrD ATOM   1557  O   SER    93     -15.700  -
1.932   7.807  1.00  0.00      BrD ATOM   1558  N   GLU    94     -16.790  -
2.194   6.298  1.00  0.00      BrD ATOM   1559  HN  GLU    94     -17.598  -
3.303   5.754  1.00  0.00      BrD ATOM   1560  CA  GLU    94     -15.729  -
4.186   6.204  1.00  0.00      BrD ATOM   1561  HA  GLU    94     -15.574  -
4.596   7.191  1.00  0.00      BrD ATOM   1562  CB  GLU    94     -16.144  -
5.314   5.258  1.00  0.00      BrD ATOM   1563  HB1 GLU    94     -16.411  -
4.887   4.302  1.00  0.00      BrD ATOM   1564  HB2 GLU    94     -17.006  -
5.817   5.671  1.00  0.00      BrD ATOM   1565  CG  GLU    94     -15.054  -
6.346   5.031  1.00  0.00      BrD ATOM   1566  HG1 GLU    94     -14.187  -
5.849   4.622  1.00  0.00      BrD ATOM   1567  HG2 GLU    94     -14.787  -
6.793   5.981  1.00  0.00      BrD ATOM   1568  CD  GLU    94     -15.479  -

7.446   4.078  1.00  0.00      BrD ATOM   1569  OE1 GLU    94     -16.617  -
7.382   3.568  1.00  0.00      BrD ATOM   1570  OE2 GLU    94     -14.673  -
8.370   3.840  1.00  0.00      BrD ATOM   1571  C   GLU    94     -14.422  -
3.556   5.725  1.00  0.00      BrD ATOM   1572  O   GLU    94     -13.351  -
4.143   5.876  1.00  0.00      BrD ATOM   1573  N   TYR    95     -14.510  -
2.357   5.150  1.00  0.00      BrD ATOM   1574  HN  TYR    95     -15.387  -
1.930   5.057  1.00  0.00      BrD ATOM   1575  CA  TYR    95     -13.227  -
1.658   4.663  1.00  0.00      BrD ATOM   1576  HA  TYR    95     -12.919  -
2.227   3.841  1.00  0.00      BrD ATOM   1577  CB  TYR    95     -13.706  -
0.260   4.166  1.00  0.00      BrD ATOM   1578  HB1 TYR    95     -14.448
0.160   4.827  1.00  0.00      BrD ATOM   1579  HB2 TYR    95     -12.825
0.367   4.176  1.00  0.00      BrD ATOM   1580  CG  TYR    95     -14.270  -
0.244   2.762  1.00  0.00      BrD ATOM   1581  CD1 TYR    95     -14.933  -
1.350   2.245  1.00  0.00      BrD ATOM   1582  HD1 TYR    95     -15.041  -
2.232   2.859  1.00  0.00      BrD ATOM   1583  CD2 TYR    95     -14.141
0.880   1.956  1.00  0.00      BrD ATOM   1584  HD2 TYR    95     -13.630
1.749   2.343  1.00  0.00      BrD ATOM   1585  CE1 TYR    95     -15.450  -
1.337   0.963  1.00  0.00      BrD ATOM   1586  HE1 TYR    95     -15.961  -
2.208   0.579  1.00  0.00      BrD ATOM   1587  CE2 TYR    95     -14.656
0.901   0.673  1.00  0.00      BrD ATOM   1588  HE2 TYR    95     -14.546
1.785   0.062  1.00  0.00      BrD ATOM   1589  CZ  TYR    95     -15.310  -
0.210   0.182  1.00  0.00      BrD ATOM   1590  OH  TYR    95     -15.823  -
0.193  -1.095  1.00  0.00      BrD ATOM   1591  HH  TYR    95     -16.730  -
0.508  -1.079  1.00  0.00      BrD ATOM   1592  C   TYR    95     -12.274  -
1.552   5.761  1.00  0.00      BrD ATOM   1593  O   TYR    95     -11.076  -
1.511   5.485  1.00  0.00      BrD ATOM   1594  N   TYR    96     -12.733  -
1.513   7.007  1.00  0.00      BrD ATOM   1595  HN  TYR    96     -13.700  -
1.553   7.161  1.00  0.00      BrD ATOM   1596  CA  TYR    96     -11.835  -
1.421   8.152  1.00  0.00      BrD ATOM   1597  HA  TYR    96     -11.033  -
0.746   7.889  1.00  0.00      BrD ATOM   1598  CB  TYR    96     -12.861  -
0.860   9.365  1.00  0.00      BrD ATOM   1599  HB1 TYR    96     -13.397  -
1.522   9.615  1.00  0.00      BrD ATOM   1600  HB2 TYR    96     -12.977
0.114   9.116  1.00  0.00      BrD ATOM   1601  CG  TYR    96     -11.712  -
0.708  10.594  1.00  0.00      BrD ATOM   1602  CD1 TYR    96     -10.351  -
0.458  10.477  1.00  0.00      BrD ATOM   1603  HD1 TYR    96      -9.918  -
0.375   9.493  1.00  0.00      BrD ATOM   1604  CD2 TYR    96     -12.252  -
0.615  11.870  1.00  0.00      BrD ATOM   1605  HD2 TYR    96     -13.308  -
1.009  11.979  1.00  0.00      BrD ATOM   1606  CE1 TYR    96      -9.551  -
0.319  11.594  1.00  0.00      BrD ATOM   1607  HE1 TYR    96      -8.495  -
0.125  11.480  1.00  0.00      BrD ATOM   1608  CE2 TYR    96     -11.458  -
0.677  12.993  1.00  0.00      BrD ATOM   1609  HE2 TYR    96     -11.895  -
0.763  13.977  1.00  0.00      BrD ATOM   1610  CZ  TYR    96     -10.109  -
0.429  12.849  1.00  0.00      BrD ATOM   1611  OH  TYR    96      -9.315  -
0.291  13.964  1.00  0.00      BrD ATOM   1612  HH  TYR    96      -8.479  -
0.742  13.821  1.00  0.00      BrD ATOM   1613  C   TYR    96     -11.238  -
2.781   8.497  1.00  0.00      BrD ATOM   1614  O   TYR    96     -10.238  -
2.468   9.211  1.00  0.00      BrD ATOM   1615  N   LYS    97     -11.857  -
3.849   7.995  1.00  0.00      BrD ATOM   1616  HN  LYS    97     -12.650  -
3.728   7.435  1.00  0.00      BrD ATOM   1617  CA  LYS    97     -11.390  -
5.200   8.256  1.00  0.00      BrD ATOM   1618  HA  LYS    97     -11.067  -
5.248   9.285  1.00  0.00      BrD ATOM   1619  CB  LYS    97     -12.547  -
6.183   8.044  1.00  0.00      BrD ATOM   1620  HB1 LYS    97     -13.075  -
5.901   7.145  1.00  0.00      BrD ATOM   1621  HB2 LYS    97     -13.223  -
6.110   8.884  1.00  0.00      BrD ATOM   1622  CG  LYS    97     -12.130  -
7.632   7.902  1.00  0.00      BrD ATOM   1623  HG1 LYS    97     -11.934
7.826   6.862  1.00  0.00      BrD ATOM   1624  HG2 LYS    97     -11.227  -
7.795   8.487  1.00  0.00      BrD ATOM   1625  CD  LYS    97     -13.205  -
8.584   8.379  1.00  0.00      BrD ATOM   1626  HD1 LYS    97     -14.156  -
8.255   7.989  1.00  0.00      BrD ATOM   1627  HD2 LYS    97     -12.986  -
9.576   8.013  1.00  0.00      BrD ATOM   1628  CE  LYS    97     -13.282  -
8.625   9.497  1.00  0.00      BrD ATOM   1629  HE1 LYS    97     -13.091  -
7.633  10.281  1.00  0.00      BrD ATOM   1630  HE2 LYS    97     -12.527  -
9.304  10.265  1.00  0.00      BrD ATOM   1631  NZ  LYS    97     -14.617  -
9.080  10.374  1.00  0.00      BrD ATOM   1632  HZ1 LYS    97     -14.760  -
10.082  10.135  1.00  0.00     BrD ATOM   1633  HZ2 LYS    97     -15.368  -
8.517   9.926  1.00  0.00      BrD ATOM   1634  HZ3 LYS    97     -14.685  -
8.968  11.406  1.00  0.00      BrD ATOM   1635  C   LYS    97     -10.212  -
5.550   7.349  1.00  0.00      BrD ATOM   1636  O   LYS    97      -9.123  -
5.870   7.824  1.00  0.00      BrD ATOM   1637  N   CYS    98     -10.443  -
5.490   6.040  1.00  0.00      BrD ATOM   1638  HN  CYS    98     -11.334  -
5.233   5.724  1.00  0.00      BrD ATOM   1639  CA  CYS    98      -9.408  -
5.811   5.062  1.00  0.00      BrD ATOM   1640  HA  CYS    98      -9.253  -
6.879   5.086  1.00  0.00      BrD ATOM   1641  CB  CYS    98      -9.862  -
5.408   3.660  1.00  0.00      BrD ATOM   1642  HB1 CYS    98      -9.000  -
5.351   3.012  1.00  0.00      BrD ATOM   1643  HB2 CYS    98     -10.337  -
4.440   3.707  1.00  0.00      BrD ATOM   1644  SG  CYS    98     -11.036  -
6.562   2.916  1.00  0.00      BrD ATOM   1645  HG  CYS    98     -11.755  -
6.695   3.538  1.00  0.00      BrD ATOM   1646  C   CYS    98      -8.093  -
5.121   5.405  1.00  0.00      BrD ATOM   1647  O   CYS    98      -7.040  -
5.757   5.442  1.00  0.00      BrD ATOM   1648  N   ALA    99      -8.159  -
3.820   5.668  1.00  0.00      BrD ATOM   1649  HN  ALA    99      -9.028  -
3.368   5.644  1.00  0.00      BrD ATOM   1650  CA  ALA    99      -6.975  -
3.066   6.046  1.00  0.00      BrD ATOM   1651  HA  ALA    99      -6.280  -
3.066   5.216  1.00  0.00      BrD ATOM   1652  CB  ALA    99      -7.339  -
1.623   6.363  1.00  0.00      BrD ATOM   1653  HB1 ALA    99      -8.281  -
1.597   6.690  1.00  0.00      BrD ATOM   1654  HB2 ALA    99      -7.425  -
1.063   5.443  1.00  0.00      BrD ATOM   1655  HB3 ALA    99      -6.568  -
1.185   6.980  1.00  0.00      BrD ATOM   1656  C   ALA    99      -6.293  -
3.721   7.232  1.00  0.00      BrD ATOM   1657  O   ALA    99      -5.091  -
3.963   7.207  1.00  0.00      BrD ATOM   1658  N   ASN   100      -7.080  -
4.054   8.247  1.00  0.00      BrD ATOM   1659  HN  ASN   100      -8.039  -
3.848   8.199  1.00  0.00      BrD ATOM   1660  CA  ASN   100      -6.388  -
4.702   9.438  1.00  0.00      BrD ATOM   1661  HA  ASN   100      -5.922  -
3.988   9.949  1.00  0.00      BrD ATOM   1662  CB  ASN   100      -7.697  -
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5.116  10.363  1.00  0.00
4.570  10.089  1.00  0.00
6.174  10.247  1.00  0.00
4.838  11.822  1.00  0.00
3.684  12.236  1.00  0.00
5.898  12.611  1.00  0.00
6.787  12.212  1.00  0.00
5.748  13.560  1.00  0.00
5.922   9.069  1.00  0.00
6.251   9.753  1.00  0.00
6.587   7.981  1.00  0.00
6.277   7.481  1.00  0.00
7.777   7.524  1.00  0.00
8.370   8.394  1.00  0.00
8.636   6.594  1.00  0.00
8.061   5.705  1.00  0.00
8.996   7.290  1.00  0.00
8.090   7.513  1.00  0.00
9.516   8.212  1.00  0.00
9.894   6.177  1.00  0.00
10.659  5.902  1.00  0.00
10.244  7.001  1.00  0.00
9.673   5.333  1.00  0.00
9.885   6.461  1.00  0.00
10.406  7.109  1.00  0.00
10.404  5.922  1.00  0.00
9.281   5.758  1.00  0.00
7.408   6.802  1.00  0.00
7.580   7.365  1.00  0.00
6.890   5.579  1.00  0.00
6.770   5.196  1.00  0.00
6.488   4.800  1.00  0.00
7.384   4.485  1.00  0.00
5.690   3.565  1.00  0.00
5.734   3.485  1.00  0.00
4.661   3.717  1.00  0.00
6.166   2.236  1.00  0.00
5.394   1.493  1.00  0.00
7.417   1.745  1.00  0.00
7.803   2.533  1.00  0.00
8.165   1.468  1.00  0.00
7.170   0.887  1.00  0.00
6.418   2.376  1.00  0.00
7.481   2.412  1.00  0.00
5.959   3.285  1.00  0.00
5.992   1.529  1.00  0.00
5.649   5.649  1.00  0.00
5.770   5.546  1.00  0.00
4.792   6.486  1.00  0.00
4.747   6.528  1.00  0.00
3.948   7.369  1.00  0.00
3.364   6.758  1.00  0.00
3.002   8.159  1.00  0.00
2.297   7.475  1.00  0.00
3.579   8.627  1.00  0.00
2.222   9.242  1.00  0.00
2.611  10.205  1.00  0.00
2.356   9.112  1.00  0.00
0.740   9.200  1.00  0.00
0.077  10.251  1.00  0.00
0.242   8.117  1.00  0.00
4.408   8.322  1.00  0.00
4.759   8.317  1.00  0.00
5.627   9.114  1.00  0.00
5.629   9.066  1.00  0.00
6.511  10.062  1.00  0.00
5.894  10.792  1.00  0.00
7.395  10.777  1.00  0.00
7.479  10.157  1.00  0.00
8.377  10.917  1.00  0.00
6.861  12.136  1.00  0.00
7.445  12.497  1.00  0.00
6.951  12.822  1.00  0.00
5.401  12.056  1.00  0.00
5.059  11.039  1.00  0.00
4.819  12.712  1.00  0.00
5.210  13.469  1.00  0.00
5.002  11.567  1.00  0.00
6.120  13.930  1.00  0.00
4.085  13.432  1.00  0.00
4.384  14.236  1.00  0.00
3.277  12.964  1.00  0.00
3.765  13.788  1.00  0.00
7.383   9.357  1.00  0.00
7.678   9.910  1.00  0.00
7.796   8.135  1.00  0.00
7.528   7.749  1.00  0.00
8.636   7.352  1.00  0.00
9.385   8.011  1.00  0.00
9.331   6.228  1.00  0.00
9.569   5.426  1.00  0.00
8.662   5.657  1.00  0.00
10.404  6.658  1.00  0.00
11.559  7.301  1.00  0.00

BrD ATOM  1663  HB1 ASN  100   -8.587
BrD ATOM  1664  HB2 ASN  100   -7.879
BrD ATOM  1665  CG  ASN  100   -7.395
BrD ATOM  1666  OD1 ASN  100   -7.283
BrD ATOM  1667  ND2 ASN  100   -7.266
BrD ATOM  1668 HD21 ASN  100   -7.370
BrD ATOM  1669 HD22 ASN  100   -7.072
BrD ATOM  1670  C   ASN  100   -5.711
BrD ATOM  1671  O   ASN  100   -4.740
BrD ATOM  1672  N   ILE  101   -6.088
BrD ATOM  1673  HN  ILE  101   -6.870
BrD ATOM  1674  CA  ILE  101   -5.377
BrD ATOM  1675  HA  ILE  101   -5.132
BrD ATOM  1676  CB  ILE  101   -6.254
BrD ATOM  1677  HB  ILE  101   -6.469
BrD ATOM  1678  CG1 ILE  101   -7.569
BrD ATOM  1679 HG11 ILE  101   -8.112
BrD ATOM  1680 HG12 ILE  101   -7.350
BrD ATOM  1681  CG2 ILE  101   -5.509
BrD ATOM  1682 HG21 ILE  101   -6.221
BrD ATOM  1683 HG22 ILE  101   -4.905
BrD ATOM  1684 HG23 ILE  101   -4.874
BrD ATOM  1685  CD1 ILE  101   -8.470
BrD ATOM  1686 HD11 ILE  101   -9.158
BrD ATOM  1687 HD12 ILE  101   -7.869
BrD ATOM  1688 HD13 ILE  101   -9.024
BrD ATOM  1689  C   ILE  101   -4.064
BrD ATOM  1690  O   ILE  101   -2.993
BrD ATOM  1691  N   LEU  102   -4.206
BrD ATOM  1692  HN  LEU  102   -5.100
BrD ATOM  1693  CA  LEU  102   -3.033
BrD ATOM  1694  HA  LEU  102   -2.519
BrD ATOM  1695  CB  LEU  102   -3.454
BrD ATOM  1696  HB1 LEU  102   -4.530
BrD ATOM  1697  HB2 LEU  102   -3.164
BrD ATOM  1698  CG  LEU  102   -2.852
BrD ATOM  1699  HG  LEU  102   -2.990
BrD ATOM  1700  CD1 LEU  102   -3.570
BrD ATOM  1701 HD11 LEU  102   -4.201
BrD ATOM  1702 HD12 LEU  102   -2.843
BrD ATOM  1703 HD13 LEU  102   -4.180
BrD ATOM  1704  CD2 LEU  102   -1.353
BrD ATOM  1705 HD21 LEU  102   -1.167
BrD ATOM  1706 HD22 LEU  102   -0.992
BrD ATOM  1707 HD23 LEU  102   -0.833
BrD ATOM  1708  C   LEU  102   -2.087
BrD ATOM  1709  O   LEU  102   -0.868
BrD ATOM  1710  N   GLU  103   -2.661
BrD ATOM  1711  HN  GLU  103   -3.639
BrD ATOM  1712  CA  GLU  103   -1.872
BrD ATOM  1713  HA  GLU  103   -1.199
BrD ATOM  1714  CB  GLU  103   -2.781
BrD ATOM  1715  HB1 GLU  103   -3.230
BrD ATOM  1716  HB2 GLU  103   -3.559
BrD ATOM  1717  CG  GLU  103   -2.060
BrD ATOM  1718  HG1 GLU  103   -2.356
BrD ATOM  1719  HG2 GLU  103   -0.999
BrD ATOM  1720  CD  GLU  103   -2.373
BrD ATOM  1721  OE1 GLU  103   -2.248
BrD ATOM  1722  OE2 GLU  103   -3.745
BrD ATOM  1723  C   GLU  103   -1.052
BrD ATOM  1724  O   GLU  103    0.175
BrD ATOM  1725  N   LYS  104   -1.740
BrD ATOM  1726  HN  LYS  104   -2.720
BrD ATOM  1727  CA  LYS  104   -1.072
BrD ATOM  1728  HA  LYS  104   -0.569
BrD ATOM  1729  CB  LYS  104   -2.097
BrD ATOM  1730  HB1 LYS  104   -2.976
BrD ATOM  1731  HB2 LYS  104   -1.670
BrD ATOM  1732  CG  LYS  104   -3.520
BrD ATOM  1733  HG1 LYS  104   -3.354
BrD ATOM  1734  HG2 LYS  104   -1.691
BrD ATOM  1735  CD  LYS  104   -2.938
BrD ATOM  1736  HD1 LYS  104   -2.817
BrD ATOM  1737  HD2 LYS  104   -2.306
BrD ATOM  1738  CE  LYS  104   -4.387
BrD ATOM  1739  HE1 LYS  104   -4.975
BrD ATOM  1740  HE2 LYS  104   -4.741
BrD ATOM  1741  NZ  LYS  104   -4.567
BrD ATOM  1742  HZ1 LYS  104   -5.135
BrD ATOM  1743  HZ2 LYS  104   -5.004
BrD ATOM  1744  HZ3 LYS  104   -3.618
BrD ATOM  1745  C   LYS  104   -0.039
BrD ATOM  1746  O   LYS  104    1.021
BrD ATOM  1747  N   PHE  105   -0.357
BrD ATOM  1748  HN  PHE  105   -1.217
BrD ATOM  1749  CA  PHE  105    0.541
BrD ATOM  1750  HA  PHE  105    0.954
BrD ATOM  1751  CB  PHE  105   -0.229
BrD ATOM  1752  HB1 PHE  105    0.455
BrD ATOM  1753  HB2 PHE  105   -0.992
BrD ATOM  1754  CG  PHE  105   -0.899
BrD ATOM  1755  CD1 PHE  105   -0.202
BrD ATOM  1756  HD1 PHE  105    0.833

11.381  7.633  1.00  0.00
10.844  6.342  1.00  0.00
10.106  5.780  1.00  0.00
12.730  7.780  1.00  0.00
13.467  8.342  1.00  0.00
12.013  6.738  1.00  0.00
12.188  6.485  1.00  0.00
12.958  7.458  1.00  0.00
13.873  7.768  1.00  0.00
7.817   6.766  1.00  0.00
7.998   7.133  1.00  0.00
6.917   5.849  1.00  0.00
6.824   5.595  1.00  0.00
6.075   5.202  1.00  0.00
6.711   4.579  1.00  0.00
5.021   4.325  1.00  0.00
5.512   3.644  1.00  0.00
4.341   4.954  1.00  0.00
4.213   3.510  1.00  0.00
4.836   2.649  1.00  0.00
5.913   2.565  1.00  0.00
2.831   3.612  1.00  0.00
2.333   4.279  1.00  0.00
4.098   1.898  1.00  0.00
4.598   1.229  1.00  0.00
2.086   2.857  1.00  0.00
1.010   2.946  1.00  0.00
2.721   2.005  1.00  0.00
2.142   1.417  1.00  0.00
5.388   6.230  1.00  0.00
5.637   6.282  1.00  0.00
4.516   7.043  1.00  0.00
4.149   6.948  1.00  0.00
3.784   8.058  1.00  0.00
3.076   7.543  1.00  0.00
3.014   8.995  1.00  0.00
3.692   9.384  1.00  0.00
2.618   9.817  1.00  0.00
1.858   8.345  1.00  0.00
0.971   9.117  1.00  0.00
1.118  10.186  1.00  0.00
1.652   6.972  1.00  0.00
2.334   6.357  1.00  0.00
0.095   8.537  1.00  0.00
0.776   9.151  1.00  0.00
0.588   6.387  1.00  0.00
0.439   5.318  1.00  0.00
0.286   7.171  1.00  0.00
1.118   6.718  1.00  0.00
4.727   8.867  1.00  0.00
4.345   9.312  1.00  0.00
5.960   9.054  1.00  0.00
6.218   8.654  1.00  0.00
6.959   9.773  1.00  0.00
6.503  10.678  1.00  0.00
8.166  10.136  1.00  0.00
7.864  10.848  1.00  0.00
8.546   9.245  1.00  0.00
9.200  10.711  1.00  0.00
9.739  10.014  1.00  0.00
7.395   8.915  1.00  0.00
7.618   9.413  1.00  0.00
7.475   7.613  1.00  0.00
7.256   7.283  1.00  0.00
7.819   6.656  1.00  0.00
8.679   7.032  1.00  0.00
8.163   5.306  1.00  0.00
7.922   5.340  1.00  0.00
7.566   4.542  1.00  0.00
9.626   4.926  1.00  0.00
9.811   4.026  1.00  0.00
9.844   4.748  1.00  0.00
10.535  6.029  1.00  0.00
10.864  6.629  1.00  0.00
9.981   6.646  1.00  0.00
11.751  5.462  1.00  0.00
11.869  4.438  1.00  0.00
11.575  5.491  1.00  0.00
12.986  6.235  1.00  0.00
13.148  6.254  1.00  0.00
13.808  5.795  1.00  0.00
12.892  7.212  1.00  0.00
6.653   6.504  1.00  0.00
6.842   6.426  1.00  0.00
5.441   6.492  1.00  0.00
5.363   6.581  1.00  0.00
4.223   6.407  1.00  0.00
4.138   5.405  1.00  0.00
2.973   6.692  1.00  0.00
3.087   7.671  1.00  0.00
2.844   5.654  1.00  0.00
3.811   5.511  1.00  0.00
2.183   6.026  1.00  0.00
1.722   6.712  1.00  0.00

BrD ATOM  1757  CD2 PHE  105   -2.226
BrD ATOM  1758  HD2 PHE  105   -2.779
BrD ATOM  1759  CE1 PHE  105   -0.816
BrD ATOM  1760  HE1 PHE  105   -0.262
BrD ATOM  1761  CE2 PHE  105   -2.846
BrD ATOM  1762  HE2 PHE  105   -3.881
BrD ATOM  1763  CZ  PHE  105   -2.140
BrD ATOM  1764  HZ  PHE  105   -2.623
BrD ATOM  1765  C   PHE  105    1.684
BrD ATOM  1766  O   PHE  105    2.845
BrD ATOM  1767  N   PHE  106    1.347
BrD ATOM  1768  HN  PHE  106    0.405
BrD ATOM  1769  CA  PHE  106    2.344
BrD ATOM  1770  HA  PHE  106    2.956
BrD ATOM  1771  CB  PHE  106    1.665
BrD ATOM  1772 HB1 PHE  106    0.985
BrD ATOM  1773 HB2 PHE  106    1.110
BrD ATOM  1774  CG  PHE  106    2.633
BrD ATOM  1775  CD1 PHE  106    3.519
BrD ATOM  1776  HD1 PHE  106    3.508
BrD ATOM  1777  CD2 PHE  106    2.662
BrD ATOM  1778  HD2 PHE  106    1.974
BrD ATOM  1779  CE1 PHE  106    4.413
BrD ATOM  1780  HE1 PHE  106    5.098
BrD ATOM  1781  CE2 PHE  106    3.548
BrD ATOM  1782  HE2 PHE  106    3.562
BrD ATOM  1783  CZ  PHE  106    4.432
BrD ATOM  1784  HZ  PHE  106    5.127
BrD ATOM  1785  C   PHE  106    3.236
BrD ATOM  1786  O   PHE  106    4.439
BrD ATOM  1787  N   PHE  107    2.643
BrD ATOM  1788  HN  PHE  107    1.679
BrD ATOM  1789  CA  PHE  107    3.401
BrD ATOM  1790  HA  PHE  107    4.035
BrD ATOM  1791  CB  PHE  107    2.462
BrD ATOM  1792 HB1 PHE  107    1.719
BrD ATOM  1793 HB2 PHE  107    3.040
BrD ATOM  1794  CG  PHE  107    1.741
BrD ATOM  1795  CD1 PHE  107    1.007
BrD ATOM  1796  HD1 PHE  107    0.954
BrD ATOM  1797  CD2 PHE  107    1.798
BrD ATOM  1798  HD2 PHE  107    2.368
BrD ATOM  1799  CE1 PHE  107    0.345
BrD ATOM  1800  HE1 PHE  107   -0.224
BrD ATOM  1801  CE2 PHE  107    1.137
BrD ATOM  1802  HE2 PHE  107    1.192
BrD ATOM  1803  CZ  PHE  107    0.410
BrD ATOM  1804  HZ  PHE  107   -0.108
BrD ATOM  1805  C   PHE  107    4.287
BrD ATOM  1806  O   PHE  107    5.369
BrD ATOM  1807  N   SER  108    3.825
BrD ATOM  1808  HN  SER  108    2.966
BrD ATOM  1809  CA  SER  108    4.607
BrD ATOM  1810  HA  SER  108    4.981
BrD ATOM  1811  CB  SER  108    3.740
BrD ATOM  1812  HB1 SER  108    2.987
BrD ATOM  1813  HB2 SER  108    3.262
BrD ATOM  1814  OG  SER  108    4.521
BrD ATOM  1815  HG  SER  108    4.902
BrD ATOM  1816  C   SER  108    5.784
BrD ATOM  1817  O   SER  108    6.887
BrD ATOM  1818  N   LYS  109    5.340
BrD ATOM  1819  HN  LYS  109    4.643
BrD ATOM  1820  CA  LYS  109    6.578
BrD ATOM  1821  HA  LYS  109    7.113
BrD ATOM  1822  CB  LYS  109    5.950
BrD ATOM  1823 HB1 LYS  109    4.898
BrD ATOM  1824 HB2 LYS  109    6.421
BrD ATOM  1825  CG  LYS  109    6.090
BrD ATOM  1826 HG1 LYS  109    5.522
BrD ATOM  1827 HG2 LYS  109    7.133
BrD ATOM  1828  CD  LYS  109    5.577
BrD ATOM  1829 HD1 LYS  109    6.413
BrD ATOM  1830 HD2 LYS  109    4.885
BrD ATOM  1831  CE  LYS  109    4.866
BrD ATOM  1832 HE1 LYS  109    5.179
BrD ATOM  1833 HE2 LYS  109    3.801
BrD ATOM  1834  NZ  LYS  109    5.175
BrD ATOM  1835 HZ1 LYS  109    6.202
BrD ATOM  1836 HZ2 LYS  109    4.715
BrD ATOM  1837 HZ3 LYS  109    4.831
BrD ATOM  1838  C   LYS  109    7.547
BrD ATOM  1839  O   LYS  109    8.761
BrD ATOM  1840  N   ILE  110    6.994
BrD ATOM  1841  HN  ILE  110    6.022
BrD ATOM  1842  CA  ILE  110    7.796
BrD ATOM  1843  HA  ILE  110    8.198
BrD ATOM  1844  CB  ILE  110    6.935
BrD ATOM  1845  HB  ILE  110    6.496
BrD ATOM  1846 CG1  ILE  110    5.811
BrD ATOM  1847 HG11 ILE  110    5.353
BrD ATOM  1848 HG12 ILE  110    5.068
BrD ATOM  1849 CG2  ILE  110    7.798
BrD ATOM  1850 HG21 ILE  110    8.756

1.945  6.264  1.00  0.00
1.401  7.732  1.00  0.00
0.938  6.152  1.00  0.00
2.345  4.297  1.00  0.00
3.133  3.583  1.00  0.00
1.985  4.366  1.00  0.00
1.540  3.971  1.00  0.00
4.274  7.411  1.00  0.00
4.045  7.060  1.00  0.00
4.582  8.662  1.00  0.00
4.752  8.875  1.00  0.00
4.664  9.730  1.00  0.00
3.660  9.972  1.00  0.00
5.308 10.972  1.00  0.00
5.373 11.743  1.00  0.00
6.304 10.718  1.00  0.00
4.542 11.528  1.00  0.00
4.204 10.718  1.00  0.00
5.162 12.252  1.00  0.00
3.252 12.203  1.00  0.00
2.701 11.525  1.00  0.00
2.666 12.417  1.00  0.00
3.527 13.485  1.00  0.00
3.698 13.239  1.00  0.00
4.411 13.952  1.00  0.00
2.389 14.442  1.00  0.00
2.656 15.356  1.00  0.00
2.127 14.593  1.00  0.00
1.565 14.066  1.00  0.00
5.465  9.289  1.00  0.00
5.112  9.407  1.00  0.00
6.549  8.561  1.00  0.00
6.780  8.364  1.00  0.00
7.407  8.085  1.00  0.00
7.588  8.914  1.00  0.00
8.745  7.600  1.00  0.00
8.589  6.661  1.00  0.00
9.432  7.445  1.00  0.00
9.383  8.573  1.00  0.00
9.856  9.367  1.00  0.00
8.611  8.987  1.00  0.00
10.425  7.912  1.00  0.00
10.932  6.837  1.00  0.00
10.734  8.468  1.00  0.00
6.729  6.960  1.00  0.00
7.120  6.677  1.00  0.00
5.744  6.318  1.00  0.00
5.486  6.579  1.00  0.00
5.046  5.216  1.00  0.00
5.620  4.936  1.00  0.00
4.989  4.008  1.00  0.00
5.914  3.455  1.00  0.00
4.166  3.373  1.00  0.00
4.848  4.336  1.00  0.00
3.645  5.624  1.00  0.00
3.035  4.943  1.00  0.00
3.146  6.743  1.00  0.00
3.676  7.255  1.00  0.00
1.836  7.229  1.00  0.00
1.732  8.253  1.00  0.00
1.749  7.200  1.00  0.00
0.695  6.414  1.00  0.00
0.085  5.813  1.00  0.00
0.590  6.405  1.00  0.00
1.231  6.921  1.00  0.00
0.482  5.683  1.00  0.00
1.195  5.369  1.00  0.00
0.066  4.443  1.00  0.00
0.563  4.768  1.00  0.00
0.773  3.824  1.00  0.00
1.047  3.570  1.00  0.00
1.000  2.565  1.00  0.00
2.469  4.061  1.00  0.00
3.149  3.228  1.00  0.00
2.571  4.493  1.00  0.00
2.699  4.804  1.00  0.00
0.683  3.517  1.00  0.00
1.397  4.094  1.00  0.00
0.306  3.924  1.00  0.00
0.701  2.491  1.00  0.00
1.193  6.603  1.00  0.00
1.183  7.823  1.00  0.00
1.801  6.018  1.00  0.00
1.787  5.043  1.00  0.00
2.516  6.794  1.00  0.00
3.470  7.083  1.00  0.00
2.786  5.956  1.00  0.00
3.218  6.606  1.00  0.00
1.480  5.367  1.00  0.00
1.713  4.570  1.00  0.00
0.904  4.968  1.00  0.00
3.786  4.850  1.00  0.00
4.261  4.538  1.00  0.00
3.371  4.010  1.00  0.00

BrD ATOM  1851 HG22 ILE  110    7.944
BrD ATOM  1852 HG23 ILE  110    7.311
BrD ATOM  1853  CD1 ILE  110    6.269
BrD ATOM  1854 HD11 ILE  110    6.222
BrD ATOM  1855 HD12 ILE  110    7.283
BrD ATOM  1856 HD13 ILE  110    5.623
BrD ATOM  1857  C   ILE  110    8.948
BrD ATOM  1858  O   ILE  110   10.104
BrD ATOM  1859  N   LYS  111    8.615
BrD ATOM  1860  HN  LYS  111    7.674
BrD ATOM  1861  CA  LYS  111    9.608
BrD ATOM  1862  HA  LYS  111    9.919
BrD ATOM  1863  CB  LYS  111    8.989
BrD ATOM  1864 HB1 LYS  111    9.742
BrD ATOM  1865 HB2 LYS  111    8.661
BrD ATOM  1866  CG  LYS  111    7.801
BrD ATOM  1867 HG1 LYS  111    7.127
BrD ATOM  1868 HG2 LYS  111    7.293
BrD ATOM  1869  CD  LYS  111    8.237
BrD ATOM  1870 HD1 LYS  111    8.872
BrD ATOM  1871 HD2 LYS  111    7.361
BrD ATOM  1872  CE  LYS  111    9.006
BrD ATOM  1873 HE1 LYS  111   10.044
BrD ATOM  1874 HE2 LYS  111    8.597
BrD ATOM  1875  NZ  LYS  111    8.916
BrD ATOM  1876 HZ1 LYS  111    9.335
BrD ATOM  1877 HZ2 LYS  111    7.921
BrD ATOM  1878 HZ3 LYS  111    9.428
BrD ATOM  1879  C   LYS  111   10.028
BrD ATOM  1880  O   LYS  111   11.964
BrD ATOM  1881  N   GLU  112   10.585
BrD ATOM  1882  HN  GLU  112    9.658
BrD ATOM  1883  CA  GLU  112   11.662
BrD ATOM  1884  HA  GLU  112   12.320
BrD ATOM  1885  CB  GLU  112   11.098
BrD ATOM  1886 HB1 GLU  112   10.589
BrD ATOM  1887 HB2 GLU  112   11.917
BrD ATOM  1888  CG  GLU  112   10.120
BrD ATOM  1889 HG1 GLU  112   10.678
BrD ATOM  1890 HG2 GLU  112    9.489
BrD ATOM  1891  CD  GLU  112    9.240
BrD ATOM  1892 OE1 GLU  112    9.625
BrD ATOM  1893 OE2 GLU  112    8.165
BrD ATOM  1894  C   GLU  112   12.467
BrD ATOM  1895  O   GLU  112   13.583
BrD ATOM  1896  N   ALA  113   11.840
BrD ATOM  1897  HN  ALA  113   10.932
BrD ATOM  1898  CA  ALA  113   12.492
BrD ATOM  1899  HA  ALA  113   13.355
BrD ATOM  1900  CB  ALA  113   11.573
BrD ATOM  1901 HB1 ALA  113   11.649
BrD ATOM  1902 HB2 ALA  113   11.865
BrD ATOM  1903 HB3 ALA  113   10.554
BrD ATOM  1904  C   ALA  113   12.953
BrD ATOM  1905  O   ALA  113   13.778
BrD ATOM  1906  N   GLY  114   12.435
BrD ATOM  1907  HN  GLY  114   11.790
BrD ATOM  1908  CA  GLY  114   12.833
BrD ATOM  1909 HA1 GLY  114   12.506
BrD ATOM  1910 HA2 GLY  114   13.911
BrD ATOM  1911  C   GLY  114   12.252
BrD ATOM  1912  O   GLY  114   12.991
BrD ATOM  1913  N   LEU  115   10.927
BrD ATOM  1914  HN  LEU  115   10.398
BrD ATOM  1915  CA  LEU  115   10.244
BrD ATOM  1916  HA  LEU  115   10.991
BrD ATOM  1917  CB  LEU  115    9.523
BrD ATOM  1918 HB1 LEU  115    8.622
BrD ATOM  1919 HB2 LEU  115    9.240
BrD ATOM  1920  CG  LEU  115   10.312
BrD ATOM  1921  HG  LEU  115    9.929
BrD ATOM  1922 CD1 LEU  115   10.120
BrD ATOM  1923 HD11 LEU  115   10.216
BrD ATOM  1924 HD12 LEU  115    9.137
BrD ATOM  1925 HD13 LEU  115   10.868
BrD ATOM  1926 CD2 LEU  115   11.790
BrD ATOM  1927 HD21 LEU  115   12.358
BrD ATOM  1928 HD22 LEU  115   11.932
BrD ATOM  1929 HD23 LEU  115   12.127
BrD ATOM  1930  C   LEU  115    9.266
BrD ATOM  1931  O   LEU  115    9.407
BrD ATOM  1932  N   ILE  116    8.209
BrD ATOM  1933  HN  ILE  116    8.131
BrD ATOM  1934  CA  ILE  116    7.196
BrD ATOM  1935  HA  ILE  116    7.614
BrD ATOM  1936  CB  ILE  116    5.920
BrD ATOM  1937  HB  ILE  116    5.183
BrD ATOM  1938 CG1  ILE  116    5.388
BrD ATOM  1939 HG11 ILE  116    4.497
BrD ATOM  1940 HG12 ILE  116    6.209
BrD ATOM  1941 CG2  ILE  116    6.220
BrD ATOM  1942 HG21 ILE  116    5.309
BrD ATOM  1943 HG22 ILE  116    6.671
BrD ATOM  1944 HG23 ILE  116    6.914
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4.534   5.217  1.00  0.00      BrD ATOM   1945  CD1 ILE   116       4.662
0.615   6.373  1.00  0.00      BrD ATOM   1946 HD11 ILE   116       3.870
0.073   5.875  1.00  0.00      BrD ATOM   1947 HD12 ILE   116       4.240
1.238   7.147  1.00  0.00      BrD ATOM   1948 HD13 ILE   116       5.356 -
0.086   4.812  1.00  0.00      BrD ATOM   1949  C   ILE   116       6.802
1.751   8.053  1.00  0.00      BrD ATOM   1950  O   ILE   116       7.024
0.544   8.154  1.00  0.00      BrD ATOM   1951  N   ASP   117       6.222
2.465   9.014  1.00  0.00      BrD ATOM   1952  HN  ASP   117       6.079
3.424   8.874  1.00  0.00      BrD ATOM   1953  CA  ASP   117       5.805
1.862  10.275  1.00  0.00      BrD ATOM   1954  HA  ASP   117       5.197
2.565  10.798  1.00  0.00      BrD ATOM   1955  CB  ASP   117       4.967
0.609  10.013  1.00  0.00      BrD ATOM   1956 HB1 ASP   117       5.564 -
0.267  10.220  1.00  0.00      BrD ATOM   1957 HB2 ASP   117       4.664
0.596   8.976  1.00  0.00      BrD ATOM   1958  CG  ASP   117       3.722
0.555  10.876  1.00  0.00      BrD ATOM   1959 OD1 ASP   117       2.897
1.488  10.787  1.00  0.00      BrD ATOM   1960 OD2 ASP   117       3.572 -
0.421  11.641  1.00  0.00      BrD ATOM   1961  C   ASP   117       7.006
1.506  11.154  1.00  0.00      BrD ATOM   1962  O   ASP   117       6.846
0.892  12.209  1.00  0.00      BrD ATOM   1963  N   LYS   118       8.206
1.897  10.725  1.00  0.00      BrD ATOM   1964  HN  LYS   118       8.282
2.384   9.679  1.00  0.00      BrD ATOM   1965  CA  LYS   118       9.416
1.613  11.488  1.00  0.00      BrD ATOM   1966  HA  LYS   118      10.248
2.063  10.968  1.00  0.00      BrD ATOM   1967  CB  LYS   118       9.315
2.220  12.889  1.00  0.00      BrD ATOM   1968 HB1 LYS   118       8.636
1.624  13.480  1.00  0.00      BrD ATOM   1969 HB2 LYS   118      10.292
2.199  13.349  1.00  0.00      BrD ATOM   1970  CG  LYS   118       8.818
3.656  12.895  1.00  0.00      BrD ATOM   1971 HG1 LYS   118       7.921
3.719  12.296  1.00  0.00      BrD ATOM   1972 HG2 LYS   118       8.595
3.946  13.911  1.00  0.00      BrD ATOM   1973  CD  LYS   118       9.857
4.408  12.327  1.00  0.00      BrD ATOM   1974 HD1 LYS   118      10.477
4.972  13.133  1.00  0.00      BrD ATOM   1975 HD2 LYS   118      10.468
4.078  11.613  1.00  0.00      BrD ATOM   1976  CE  LYS   118       9.208
5.796  11.631  1.00  0.00      BrD ATOM   1977 HE1 LYS   118       8.502
5.425  10.902  1.00  0.00      BrD ATOM   1978 HE2 LYS   118       8.687
6.386  12.369  1.00  0.00      BrD ATOM   1979  NZ  LYS   118      10.212
6.652  10.943  1.00  0.00      BrD ATOM   1980 HZ1 LYS   118      11.163
6.458  11.316  1.00  0.00      BrD ATOM   1981 HZ2 LYS   118       9.989
7.656  11.036  1.00  0.00      BrD ATOM   1982 HZ3 LYS   118      10.206
6.459   9.921  1.00  0.00      BrD ATOM   1983  C   LYS   118       9.657
0.110  11.591  1.00  0.00      BrD ATOM   1984 OT1 LYS   118       9.047 -
0.641  10.802  1.00  0.00      BrD ATOM   1985 OT2 LYS   118      10.454 -
0.302  12.459  1.00  0.00      BrD END
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